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DATE: Wednesday, December 12, 2007

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**Hit Count**

*DB=PGPB,USPT; PLUR=YES; OP=ADJ*

<input type="checkbox"/>	L4	(pyrrolo adj3 pyridazine)	8
<input type="checkbox"/>	L3	L2 and (pyrrolo adj3 pyridazine)	0
<input type="checkbox"/>	L2	514/525.06.icls. or 514/252.06.ccls. or 544/236.icls. or 544/236.ccls.	910
<input type="checkbox"/>	L1	6342601.pn.	1

END OF SEARCH HISTORY

FILE 'REGISTRY' ENTERED AT 10:19:12 ON 12 DEC 2007  
L1                   STRUCTURE uploaded  
L2                   0 S L1  
L3                   237 S L1 SSS FULL

FILE 'CAPLUS' ENTERED AT 10:21:22 ON 12 DEC 2007  
L4                   7 S L3

FILE 'REGISTRY' ENTERED AT 10:28:45 ON 12 DEC 2007  
L5                   STRUCTURE uploaded  
L6                   1 S L5  
L7                   86 S L5 SSS FULL

FILE 'CAPLUS' ENTERED AT 10:29:37 ON 12 DEC 2007  
L8                   19 S L7  
L9                   18 S L8 NOT L4

FILE 'REGISTRY' ENTERED AT 11:33:03 ON 12 DEC 2007  
L10                  STRUCTURE uploaded  
L11                  3 S L10  
L12                  54 S L10 SSS FULL

FILE 'CAPLUS' ENTERED AT 11:36:06 ON 12 DEC 2007  
L13                  4 S L12

=> file registry	SINCE FILE	TOTAL
COST IN U.S. DOLLARS	ENTRY	SESSION
FULL ESTIMATED COST	0.21	0.21

FILE 'REGISTRY' ENTERED AT 10:19:12 ON 12 DEC 2007  
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STRUCTURE FILE UPDATES: 11 DEC 2007 HIGHEST RN 957570-32-0  
DICTIONARY FILE UPDATES: 11 DEC 2007 HIGHEST RN 957570-32-0

New CAS Information Use Policies, enter HELP USAGETERMS for details.

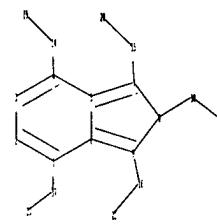
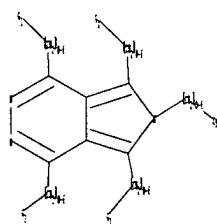
TSCA INFORMATION NOW CURRENT THROUGH June 29, 2007

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conducting SmartSELECT searches.

REGISTRY includes numerically searchable data for experimental and  
predicted properties as well as tags indicating availability of  
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<http://www.cas.org/support/stngen/stndoc/properties.html>

=>  
Uploading C:\Program Files\Stnexp\Queries\10520962broad.str



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ring nodes :
1 2 3 4 5 6 7 8 9
chain bonds :
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ring bonds :
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exact/norm bonds :
1-2 1-6 2-3 3-4 4-5 5-6 5-7 6-9 7-8 8-9 10-11 14-19 15-20 16-22 17-23

exact bonds :
1-17 4-14 7-15 8-10 9-16
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G1:H,Cy

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Match level :
1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 6:Atom 7:Atom 8:Atom 9:Atom 10:CLASS
11:Atom 14:CLASS 15:CLASS 16:CLASS 17:CLASS 19:CLASS 20:CLASS 22:CLASS
23:CLASS
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L1 STRUCTURE UPLOADED

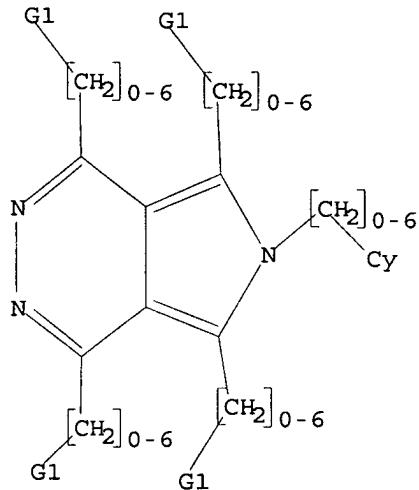
=> s 11  
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SAMPLE SCREEN SEARCH COMPLETED - 78197 TO ITERATE

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INCOMPLETE SEARCH (SYSTEM LIMIT EXCEEDED)  
SEARCH TIME: 00.00.01

FULL FILE PROJECTIONS: ONLINE \*\*INCOMPLETE\*\*  
BATCH \*\*INCOMPLETE\*\*  
PROJECTED ITERATIONS: 1547303 TO 1580577  
PROJECTED ANSWERS: 0 TO 0

L2 0 SEA SSS SAM L1

=> d 11  
L1 HAS NO ANSWERS  
L1 STR



G1 H, CY

Structure attributes must be viewed using STN Express query preparation.

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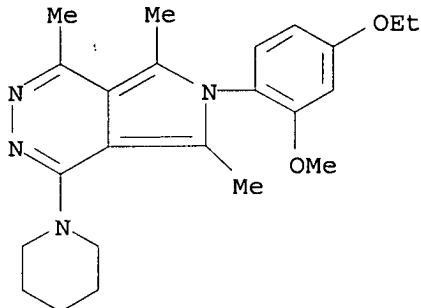
64.2% PROCESSED 1000000 ITERATIONS 237 ANSWERS  
INCOMPLETE SEARCH (SYSTEM LIMIT EXCEEDED)  
SEARCH TIME: 00.00.16

FULL FILE PROJECTIONS: ONLINE \*\*INCOMPLETE\*\*  
BATCH \*\*INCOMPLETE\*\*  
PROJECTED ITERATIONS: 1557677 TO 1557677  
PROJECTED ANSWERS: 312 TO 426

L3 237 SEA SSS FUL L1

=> d 13 scan

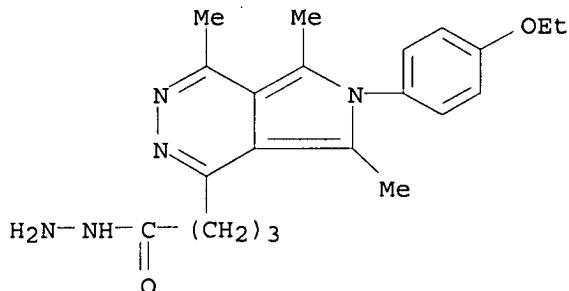
L3 237 ANSWERS REGISTRY COPYRIGHT 2007 ACS on STN  
IN 6H-Pyrrolo[3,4-d]pyridazine, 6-(4-ethoxy-2-methoxyphenyl)-1,5,7-trimethyl-  
4-(1-piperidinyl)-  
MF C23 H30 N4 O2



\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

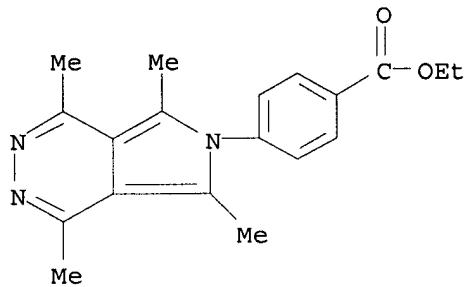
HOW MANY MORE ANSWERS DO YOU WISH TO SCAN? (1):3

L3 237 ANSWERS REGISTRY COPYRIGHT 2007 ACS on STN  
IN 6H-Pyrrolo[3,4-d]pyridazine-1-butanoic acid, 6-(4-ethoxyphenyl)-4,5,7-  
trimethyl-, hydrazide  
MF C21 H27 N5 O2



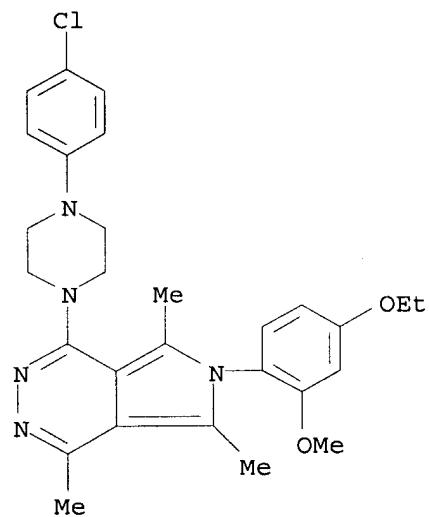
\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

L3 237 ANSWERS REGISTRY COPYRIGHT 2007 ACS on STN  
IN Benzoic acid, 4-(1,4,5,7-tetramethyl-6H-pyrrolo[3,4-d]pyridazin-6-yl)-,  
ethyl ester  
MF C19 H21 N3 O2



\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

L3 237 ANSWERS REGISTRY COPYRIGHT 2007 ACS on STN  
 IN 6H-Pyrrolo[3,4-d]pyridazine, 1-[4-(4-chlorophenyl)-1-piperazinyl]-6-(4-  
 ethoxy-2-methoxyphenyl)-4,5,7-trimethyl-  
 MF C28 H32 Cl N5 O2



\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

HOW MANY MORE ANSWERS DO YOU WISH TO SCAN? (1):0

=> file caplus		SINCE FILE	TOTAL
COST IN U.S. DOLLARS		ENTRY	SESSION
FULL ESTIMATED COST		173.45	173.66

FILE 'CAPLUS' ENTERED AT 10:21:22 ON 12 DEC 2007  
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FILE COVERS 1907 - 12 Dec 2007 VOL 147 ISS 25  
FILE LAST UPDATED: 11 Dec 2007 (20071211/ED)

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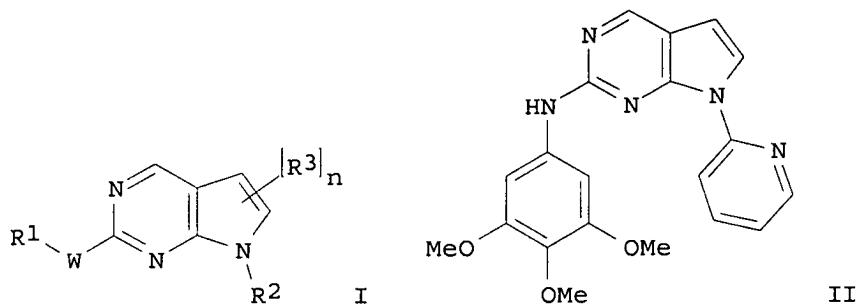
<http://www.cas.org/infopolicy.html>

=> s 13  
L4 7 L3

=> d 14 1-7 ti abs bib

L4 ANSWER 1 OF 7 CAPLUS COPYRIGHT 2007 ACS on STN  
TI Expedited SAR study of high-affinity ligands to the  $\alpha 2\delta$  subunit of voltage-gated calcium channels: Generation of a focused library using a solution-phase Sn2Ar coupling methodology  
AB The SAR of the lead compound 3, a novel ligand for the  $\alpha 2\delta$  subunit of voltage-gated calcium channels, was rapidly explored. Utilizing a parallel solution-phase Sn2Ar coupling approach, a focused library was obtained. The library was evaluated in vitro and afforded a series of analogs with improved potencies. The SAR trends of the library are also described.  
AN 2005:1342000 CAPLUS <<LOGINID::20071212>>  
DN 144:100381  
TI Expedited SAR study of high-affinity ligands to the  $\alpha 2\delta$  subunit of voltage-gated calcium channels: Generation of a focused library using a solution-phase Sn2Ar coupling methodology  
AU Chen, Chixu; Stearns, Brian; Hu, Tao; Anker, Naomi; Santini, Angelina; Arruda, Jeannie M.; Campbell, Brian T.; Datta, Purabi; Aiyar, Jayashree; Munoz, Benito  
CS Department of Chemistry, Merck Research Laboratories, San Diego, CA, 92121, USA  
SO Bioorganic & Medicinal Chemistry Letters (2006), 16(3), 746-749  
CODEN: BMCLE8; ISSN: 0960-894X  
PB Elsevier B.V.  
DT Journal  
LA English  
OS CASREACT 144:100381  
RE.CNT 24 THERE ARE 24 CITED REFERENCES AVAILABLE FOR THIS RECORD  
ALL CITATIONS AVAILABLE IN THE RE FORMAT

L4 ANSWER 2 OF 7 CAPLUS COPYRIGHT 2007 ACS on STN  
TI Preparation of substituted pyrrolo[2,3-d]pyrimidines as inducers of keratinocyte differentiation  
GI



AB The invention provides compds. I [ $n = 0-2$ ; W = NR4, S, O, SO, SO2 (wherein R4 = H, alkyl); R1 = arylalkyl, heteroarylalkyl, cycloalkylalkyl, etc.; R2 = arylalkyl, heteroarylalkyl, cycloalkylalkyl, etc.; R3 = halo, OH, XSR5, etc. (X = a bond, alkylene; R5 = H, alkyl, cycloalkylalkyl)], pharmaceutical compns. comprising such compds. and methods of using such compds. to induce undifferentiated keratinocytes to differentiate into terminally differentiated keratinocytes. The invention further provides compds. for the treatment of diseases or disorders associated with casein kinase II (CK2), TANK-binding kinase 1 (TBK1) and NIMA-related kinase 9 (NEK9). Over 200 compds. I were prepared E.g., a 4-step synthesis of II, starting from 5-bromo-2,4-dichloropyrimidine, was given.

AN 2005:1220346 CAPLUS <<LOGINID::20071212>>

DN 143:477978

TI Preparation of substituted pyrrolo[2,3-d]pyrimidines as inducers of keratinocyte differentiation

IN Hong, Jiyong; Gray, Nathanael S.; Schultz, Peter

PA IRM LLC, Bermuda

SO PCT Int. Appl., 53 pp.

CODEN: PIXXD2

DT Patent

LA English

FAN.CNT 1

	PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI	WO 2005107760	A1	20051117	WO 2005-US15118	20050429
	W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BW, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, EG, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KM, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NA, NI, NO, NZ, OM, PG, PH, PL, PT, RO, RU, SC, SD, SE, SG, SK, SL, SM, SY, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, YU, ZA, ZM, ZW				
	RW: BW, GH, GM, KE, LS, MW, MZ, NA, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IS, IT, LT, LU, MC, NL, PL, PT, RO, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG				

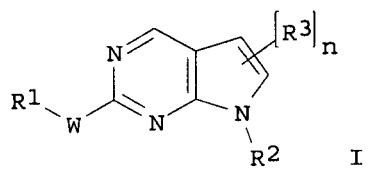
PRAI US 2004-567346P P 20040430

OS CASREACT 143:477978; MARPAT 143:477978

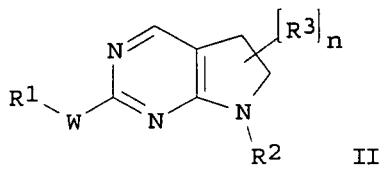
RE.CNT 1 THERE ARE 1 CITED REFERENCES AVAILABLE FOR THIS RECORD  
ALL CITATIONS AVAILABLE IN THE RE FORMAT

L4 ANSWER 3 OF 7 CAPLUS COPYRIGHT 2007 ACS on STN  
TI Preparation of pyrrolopyrimidines and their analogs as protein kinase inhibitors

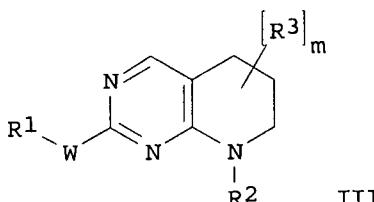
GI



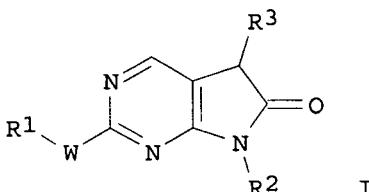
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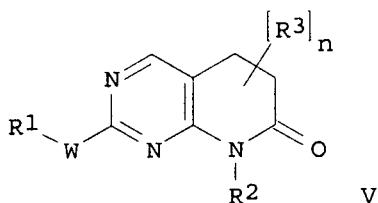
II



III



IV



V

AB The invention provides a novel class of compds. I-V [n = 0-2; m = 0-3; W = NR4, S, O, SO, SO2 (wherein R4 = H, alkyl); R1 = (un)substituted (hetero)arylalkyl, (hetero)cycloalkyl; R2 = (un)substituted (hetero)arylalkyl, (hetero)cycloalkyl; R3 = halo, OH, XSR5, etc. (X = a bond, alkylene; R5 = H, alkyl, cycloalkylalkyl)], pharmaceutical compns. comprising such compds. and methods of using such compds. to treat or prevent diseases or disorders associated with abnormal or deregulated kinase activity, particularly diseases or disorders that involve abnormal activation of the FAK, Abl, BCR-Abl, PDGF-R, c-Kit, NPM-ALK, Flt-3, JAK2 and c-Met kinases. Over 200 compds. I-V were prepared and characterized. The preparation of the compds. I is illustrated in examples. E.g., synthesis of I [R1 = 3,4,6-(MeO)3C6H2; R2 = 2-pyridyl; R3 = H; W = NH], starting from 5-bromo-2,4-dichloropyrimidine, was given. The compds. I-V were tested against various kinases. For example, they inhibit the enzyme activity by 50% (IC50), in a concentration of from 0.001 to 0.5  $\mu$ M, especially from 0.01 to 0.1  $\mu$ M.

AN 2005:962258 CAPLUS <<LOGINID::20071212>>  
DN 143:266947

TI Preparation of pyrrolopyrimidines and their analogs as protein kinase inhibitors

IN Choi, Ha-Soon; Wang, Zhicheng; Gray, Nathanael Schiander; Gu, Xiang-Ju; He, Xiaohui; He, Yun; Jiang, Tao; Liu, Yi; Richmond, Wendy; Sim, Taebo; Yang, Kunyong

PA IRM LLC, Bermuda

SO PCT Int. Appl., 63 pp.  
CODEN: PIXXD2

DT Patent

LA English

FAN.CNT 1

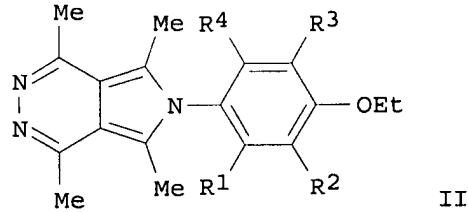
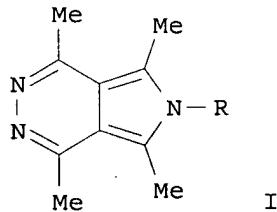
PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
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PI WO 2005080393	A1	20050901	WO 2005-US4630	20050214

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 CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, EG, ES, FI, GB, GD,  
 GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC,  
 LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NA, NI,  
 NO, NZ, OM, PG, PH, PL, PT, RO, RU, SC, SD, SE, SG, SK, SL, SY,  
 TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, YU, ZA, ZM, ZW  
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 AU 2005214352 A1 20050901 AU 2005-214352 20050214  
 CA 2553785 A1 20050901 CA 2005-2553785 20050214  
 EP 1713806 A1 20061025 EP 2005-713510 20050214  
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 CN 1918158 A 20070221 CN 2005-80004895 20050214  
 BR 2005007668 A 20070717 BR 2005-7668 20050214  
 JP 2007522241 T 20070809 JP 2006-553321 20050214  
 MX 2006PA09158 A 20061110 MX 2006-PA9158 20060811  
 IN 2006CN02987 A 20070608 IN 2006-CN2987 20060814  
 US 2007225306 A1 20070927 US 2007-589099 20070611  
 PRAI US 2004-544944P P 20040214  
 WO 2005-US4630 W 20050214  
 OS MARPAT 143:266947

RE.CNT 3 THERE ARE 3 CITED REFERENCES AVAILABLE FOR THIS RECORD  
 ALL CITATIONS AVAILABLE IN THE RE FORMAT

L4 ANSWER 4 OF 7 CAPLUS COPYRIGHT 2007 ACS on STN  
 TI Synthesis and biological evaluation of 6-aryl-6H-pyrrolo[3,4-d]pyridazine  
 derivatives as high-affinity ligands of the  $\alpha 2\delta$  subunit of  
 voltage-gated calcium channels

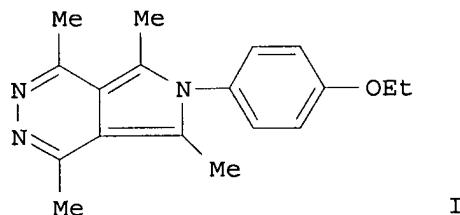
GI



AB 2H-pyrrolo[3,4-c]pyridazines I (R = 4-EtOC<sub>6</sub>H<sub>4</sub>, 2-EtO-5-pyridinyl,  
 5-EtO-2-pyridinyl, 5-EtO-2-pyrazinyl, 4-EtO-1-pyridazinyl,  
 2-EtO-5-pyrimidinyl, etc.) such as II (R<sub>1</sub> = H, MeO, Et, H<sub>2</sub>C:CH, Me, MeS,  
 EtO, F; R<sub>2</sub> = H, Me; R<sub>3</sub> = H, Me, Cl, HOCH<sub>2</sub>; R<sub>4</sub> = H, Me) are prepared as  
 ligands for the  $\alpha 2\delta$  subunit of voltage-gated calcium channels.  
 Ortho-substituents capable of electron-donation increase the binding of II  
 to the  $\alpha 2\delta$  subunit of voltage-gated calcium channels;  
 electron-withdrawing substituents in the ortho-position of II decrease  
 binding significantly. II (R<sub>1</sub> = MeO; R<sub>2</sub> = R<sub>3</sub> = R<sub>4</sub> = H) binds to the  
 $\alpha 2\delta$  subunit of voltage-gated calcium channels from A710 cells  
 with an IC<sub>50</sub> value of 4 nM. Testing of tritiated ligand II (R<sub>1</sub> = TCH<sub>2</sub>TCH;  
 R<sub>2</sub> = R<sub>3</sub> = R<sub>4</sub> = H) in purified human  $\alpha 2\delta$  voltage-gated calcium  
 channel subunits indicates that II displace Gabapentin from the  
 $\alpha 2\delta$  subunit of voltage-gated calcium channels, and thus act as  
 Gabapentin mimics *in vitro*. In the preparation of II (R<sub>1</sub> = Et; R<sub>2</sub> = R<sub>3</sub> = R<sub>4</sub> =  
 H), a novel metal-free hydrogenation is used using hydrazine as the  
 reductant; the reduction is effective in other systems (no data).

AN 2004:303255 CAPLUS <<LOGINID::20071212>>  
DN 141:54277  
TI Synthesis and biological evaluation of 6-aryl-6H-pyrrolo[3,4-d]pyridazine derivatives as high-affinity ligands of the  $\alpha 2\delta$  subunit of voltage-gated calcium channels  
AU Hu, Tao; Stearns, Brian A.; Campbell, Brian T.; Arruda, Jeannie M.; Chen, Chixu; Aiyar, Jayashree; Bezverkova, Robert E.; Santini, Angelina; Schaffhauser, Herve; Liu, Wensheng; Venkatraman, Shankar; Munoz, Benito  
CS MRLSDB2, Department of Medicinal Chemistry, Merck Research Laboratories, San Diego, CA, 92121, USA  
SO Bioorganic & Medicinal Chemistry Letters (2004), 14(9), 2031-2034  
CODEN: BMCLE8; ISSN: 0960-894X  
PB Elsevier Science B.V.  
DT Journal  
LA English  
OS CASREACT 141:54277  
RE.CNT 9 THERE ARE 9 CITED REFERENCES AVAILABLE FOR THIS RECORD  
ALL CITATIONS AVAILABLE IN THE RE FORMAT

L4 ANSWER 5 OF 7 CAPLUS COPYRIGHT 2007 ACS on STN  
TI Synthesis and biological evaluation of 6-aryl-6H-pyrrolo[3,4-d]pyridazine derivatives: high-affinity ligands to the  $\alpha 2\delta$  subunit of voltage gated calcium channels  
GI



AB A novel class of 6-aryl-6H-pyrrolo[3,4-d]pyridazine ligands for the  $\alpha 2\delta$  subunit of voltage-gated calcium channels has been described. Substitutions in the aryl ring of the mol. were generally not tolerated, and resulted in diminished binding to the  $\alpha 2\delta$  subunit. Modifications to the pyridazine ring revealed numerous permissive substitutions, and detailed SAR studies were carried out in this portion of the mol. Replacement of the pyridazine ring Me group with an aminomethyl functionality provided greatly improved potency over the initial lead. The initial lead compound (I) displayed good rat pharmacokinetic properties, and was shown to be efficacious in the Chung model for neuropathic pain in rats.

AN 2004:153601 CAPLUS <<LOGINID::20071212>>  
DN 140:357282  
TI Synthesis and biological evaluation of 6-aryl-6H-pyrrolo[3,4-d]pyridazine derivatives: high-affinity ligands to the  $\alpha 2\delta$  subunit of voltage gated calcium channels  
AU Stearns, Brian A.; Anker, Naomi; Arruda, Jeannie M.; Campbell, Brian T.; Chen, Chixu; Cramer, Merryl; Hu, Tao; Jiang, Xiaohui; Park, Kenneth; Ren, Kun Kun; Sablad, Marciano; Santini, Angelina; Schaffhauser, Herve; Urban, Mark O.; Munoz, Benito  
CS Department of Medicinal Chemistry, Merck Research Laboratories, San Diego, CA, 92121, USA  
SO Bioorganic & Medicinal Chemistry Letters (2004), 14(5), 1295-1298  
CODEN: BMCLE8; ISSN: 0960-894X

PB Elsevier Science B.V.

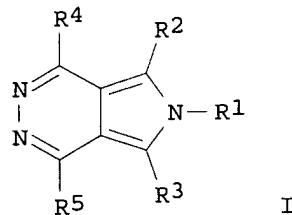
DT Journal

LA English

OS CASREACT 140:357282

RE.CNT 16 THERE ARE 16 CITED REFERENCES AVAILABLE FOR THIS RECORD  
ALL CITATIONS AVAILABLE IN THE RE FORMAT

L4 ANSWER 6 OF 7 CAPLUS COPYRIGHT 2007 ACS on STN  
TI Treatment of neuropathic pain with 6H-pyrrolo[3,4-d]pyridazine compounds  
GI



AB The title compds. [I; R1 = (un)substituted alkyl(hetero)aryl, alkyl(hetero)cycloalkyl, (hetero)aryl, (hetero)cycloalkyl; R2-R5 = a bond, (un)substituted alkyl, alkyl(hetero)aryl, alkyl(hetero)cycloalkyl, (hetero)aryl, (hetero)cycloalkyl] were prepared as ligands of voltage gated calcium channels (VGCC), useful in the treatment of neuropathic pain, and psychiatric and mood disorders such as, for example, schizophrenia, anxiety, depression, panic, and bipolar disorder, as well as in the treatment of pain, Parkinson's disease, cognitive dysfunction, epilepsy, circadian rhythm disorders, drug addiction, drug abuse, drug withdrawal and other. E.g., a multi-step synthesis of I [R1 = 4-EtOC6H4; R2-R4 = Me; R5 = 4-MeOC6H4] which produced a 65% effect after i.p. dosing at 30 mg/kg in spinal nerve ligation model of neuropathic pain in rats, was given. The pharmaceutical composition comprising the compound I is claimed.

AN 2004:60243 CAPLUS <<LOGINID::20071212>>

DN 140:111422

TI Treatment of neuropathic pain with 6H-pyrrolo[3,4-d]pyridazine compounds

IN Anker, Naomi Burke; Arruda, Jeannie M.; Campbell, Brian Thomas; Munoz, Benito; Prasit, Petpiboon; Stearns, Brian A.

PA Merck & Co., Inc., USA

SO PCT Int. Appl., 203 pp.  
CODEN: PIXXD2

DT Patent

LA English

FAN.CNT 1

	PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI	WO 2004006836	A2	20040122	WO 2003-US21493	20030708
	WO 2004006836	A3	20040415		
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 US 2006154929 A1 20060713 US 2005-520962 20051128  
 PRAI US 2002-394734P P 20020711  
 WO 2003-US21493 W 20030708  
 OS MARPAT 140:111422  
  
 L4 ANSWER 7 OF 7 CAPLUS COPYRIGHT 2007 ACS on STN  
 TI Synthesis and electrophilic substitution of dipyrrolo[1,2-b:3,4-d]pyridazines  
 AB Dipyrrolo[1,2-b:3,4-d]pyridazines were prepared from 1,4,5,7-tetramethyl-6-R1-pyrrolo[3,4-d]-pyridazines. The dipyrrolo[1,2-b:3,4-d]pyridazines were found to have high nucleophilicity and electrophilic substitution occurs at C7, or C7 and C9 depending on the steric bulk and activity of the attacking electrophile.  
 AN 2003:927977 CAPLUS <>LOGINID::20071212>>  
 DN 140:303615  
 TI Synthesis and electrophilic substitution of dipyrrolo[1,2-b:3,4-d]pyridazines  
 AU Arsen'ev, V. G.; Arsen'eva, M. Yu.; Shopin, D. V.; Olekhovich, L. P.  
 CS Rostov State University, Rostov-on-Don, 344006, Russia  
 SO Chemistry of Heterocyclic Compounds (New York, NY, United States) (Translation of Khimiya Geterotsiklicheskikh Soedinenii) (2003), 39(5), 669-670  
 CODEN: CHCCAL; ISSN: 0009-3122  
 PB Kluwer Academic/Consultants Bureau  
 DT Journal  
 LA English  
 OS CASREACT 140:303615  
 RE.CNT 4 THERE ARE 4 CITED REFERENCES AVAILABLE FOR THIS RECORD  
 ALL CITATIONS AVAILABLE IN THE RE FORMAT

=> d his

(FILE 'HOME' ENTERED AT 10:19:03 ON 12 DEC 2007)

FILE 'REGISTRY' ENTERED AT 10:19:12 ON 12 DEC 2007

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 L3 237 S L1 SSS FULL

FILE 'CAPLUS' ENTERED AT 10:21:22 ON 12 DEC 2007

L4 7 S L3

=> log hold

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FULL ESTIMATED COST	20.28	193.94
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CA SUBSCRIBER PRICE	-5.46	-5.46

SESSION WILL BE HELD FOR 120 MINUTES

STN INTERNATIONAL SESSION SUSPENDED AT 10:21:37 ON 12 DEC 2007

Connecting via Winsock to STN

Welcome to STN International! Enter x:x

LOGINID:SSPTAEX01623

PASSWORD:

\* \* \* \* \* RECONNECTED TO STN INTERNATIONAL \* \* \* \* \*  
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FILE 'CPLUS' ENTERED AT 10:28:35 ON 12 DEC 2007  
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COST IN U.S. DOLLARS	SINCE FILE ENTRY	TOTAL SESSION
FULL ESTIMATED COST	20.28	193.94
DISCOUNT AMOUNTS (FOR QUALIFYING ACCOUNTS)	SINCE FILE ENTRY	TOTAL SESSION
CA SUBSCRIBER PRICE	-5.46	-5.46
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FULL ESTIMATED COST	20.28	193.94
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CA SUBSCRIBER PRICE	-5.46	-5.46

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DICTIONARY FILE UPDATES: 11 DEC 2007 HIGHEST RN 957570-32-0

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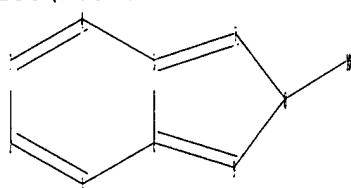
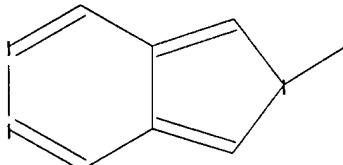
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<http://www.cas.org/support/stngen/stndoc/properties.html>

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ring nodes :
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ring bonds :
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G1:H,Cy

Match level :  
1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 6:Atom 7:Atom 8:Atom 9:Atom 10:CLASS

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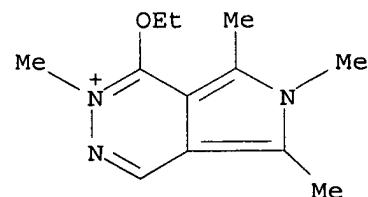
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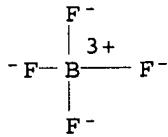
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L6 1 ANSWERS REGISTRY COPYRIGHT 2007 ACS on STN  
IN 6H-Pyrrolo[3,4-d]pyridazinium, 1-ethoxy-2,5,6,7-tetramethyl-,  
tetrafluoroborate(1-) (9CI)  
MF C12 H18 N3 O . B F4

CM 1



CM 2



ALL ANSWERS HAVE BEEN SCANNED

=> s 15 sss full  
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100.0% PROCESSED 120189 ITERATIONS 86 ANSWERS  
 SEARCH TIME: 00.00.01

L7 86 SEA SSS FUL L5

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	ENTRY	SESSION	
CA SUBSCRIBER PRICE	0.00	-5.46	

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FILE COVERS 1907 - 12 Dec 2007 VOL 147 ISS 25  
 FILE LAST UPDATED: 11 Dec 2007 (20071211/ED)

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<http://www.cas.org/infopolicy.html>

=> s 17  
 L8 19 L7

=> d 18 1-19 ti abs bib hitstr

L8 ANSWER 1 OF 19 CAPLUS COPYRIGHT 2007 ACS on STN  
 TI Synthesis of 5-aryl-2-oxopyrrole derivatives as synthons for highly substituted pyrroles  
 AB A small library of 2-oxo-5-(hetero)arylpyrroles was prepared starting from 2,3-dioxo-5-(hetero)arylpolyridines. The large synthetic possibilities

of these 2-oxopyrroles were investigated. The 2-oxopyrroles offer a large number of possible derivatizations including reactions with electrophiles. The chloroformylation of 2-oxo-5-(hetero)arylpyrroles provides pyrrole carbaldehydes. Some pyrrole carbaldehydes were used to synthesize polycyclic compds. like pyrrolo[3,4-d]pyridazinones, a thienopyrrole, a pyrrolobenz[1,4]oxazepine, a pyrrolobenz[1,4]thiazepine, and a pyrrolobenz[1,4]diazepine. Hereby we showed through a short exploration that the oxopyrroles and analogs are interesting and versatile synthetic building blocks.

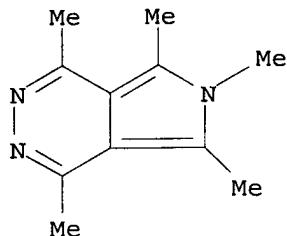
AN 2006:498781 CAPLUS <<LOGINID::20071212>>  
DN 145:167033  
TI Synthesis of 5-aryl-2-oxopyrrole derivatives as synthons for highly substituted pyrroles  
AU Metten, Bert; Kostermans, Maarten; Van Baelen, Gitte; Smet, Mario; Dehaen, Wim  
CS Department of Chemistry, Katholieke Universiteit Leuven, Louvain, B-3001, Belg.  
SO Tetrahedron (2006), 62(25), 6018-6028  
CODEN: TETRAB; ISSN: 0040-4020  
PB Elsevier B.V.  
DT Journal  
LA English  
OS CASREACT 145:167033  
IT 901764-67-8P  
RL: SPN (Synthetic preparation); PREP (Preparation)  
(synthesis of library of 5-aryl-2-oxopyrrole derivs. from  
2,3-dioxo-5-arylpyrrolidines and their use as synthons for highly  
substituted pyrroles)  
RN 901764-67-8 CAPLUS  
CN 1H-Pyrrolo[3,4-d]pyridazin-1-one, 5-chloro-2,6-dihydro-7-phenyl-6-(phenylmethyl)- (CA INDEX NAME)

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RE.CNT 31 THERE ARE 31 CITED REFERENCES AVAILABLE FOR THIS RECORD  
ALL CITATIONS AVAILABLE IN THE RE FORMAT

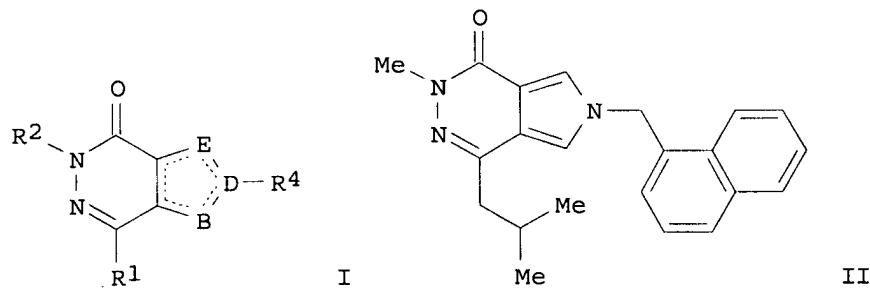
L8 ANSWER 2 OF 19 CAPLUS COPYRIGHT 2007 ACS on STN  
TI Synthesis and electrophilic substitution of dipyrrolo[1,2-b:3,4-d]pyridazines  
AB Dipyrrolo[1,2-b:3,4-d]pyridazines were prepared from 1,4,5,7-tetramethyl-6-R1-pyrrolo[3,4-d]-pyridazines. The dipyrrolo[1,2-b:3,4-d]pyridazines were found to have high nucleophilicity and electrophilic substitution occurs at C7, or C7 and C9 depending on the steric bulk and activity of the attacking electrophile.  
AN 2003:927977 CAPLUS <<LOGINID::20071212>>  
DN 140:303615  
TI Synthesis and electrophilic substitution of dipyrrolo[1,2-b:3,4-d]pyridazines  
AU Arsen'ev, V. G.; Arsen'eva, M. Yu.; Shopin, D. V.; Olekhovich, L. P.  
CS Rostov State University, Rostov-on-Don, 344006, Russia  
SO Chemistry of Heterocyclic Compounds (New York, NY, United States) (Translation of Khimiya Geterotsiklicheskikh Soedinenii) (2003), 39(5), 669-670  
CODEN: CHCCAL; ISSN: 0009-3122  
PB Kluwer Academic/Consultants Bureau  
DT Journal  
LA English  
OS CASREACT 140:303615  
IT 79398-46-2  
RL: RCT (Reactant); RACT (Reactant or reagent)  
(synthesis of dipyrrolopyridazines from pyrrolopyridazines and their reactivity in electrophilic substitution reactions)

RN 79398-46-2 CAPLUS  
CN 6H-Pyrrolo[3,4-d]pyridazine, 1,4,5,6,7-pentamethyl- (CA INDEX NAME)



RE.CNT 4 THERE ARE 4 CITED REFERENCES AVAILABLE FOR THIS RECORD  
ALL CITATIONS AVAILABLE IN THE RE FORMAT

L8 ANSWER 3 OF 19 CAPLUS COPYRIGHT 2007 ACS on STN  
TI Preparation of novel fused pyridazinones useful as immunosuppressants  
GI



AB The invention provides certain pyrrolo-, thieno-, furano- and pyrazolo[3,4-d]pyridazinones of general formula I [B = CH, N, S, or O; D = C or N; E = CR<sub>3</sub> or N; with various dependencies; R<sub>1</sub> = alkyl, alkoxy, (di)(alkyl)amino, Ph, cycloalkyl, etc.; R<sub>2</sub> = Me, alkyl, alkoxyalkyl; R<sub>3</sub> = H, (un)substituted carbamoyl, various derivs. of OH and SH; R<sub>4</sub> = (un)substituted (hetero)aryl methyl, (hetero)aryl, (hetero)arylmethyl, acenaphthenyl, indanyl, or fluorenyl] and their pharmaceutically acceptable salts or solvates. Also disclosed are processes for their preparation, pharmaceutical compns. containing them, a process

for preparing the pharmaceutical compns., and methods of treatment involving their use. In particular, their use in immunosuppression, and especially in therapy of reversible obstructive airways diseases, is claimed. For example, title compound II was prepared in 4 steps: (1) bromination of 4-methyl-2-pentanone and reaction with Ph<sub>3</sub>P:CHCO<sub>2</sub>Me to give (E)-Me 6-methyl-4-oxo-2-heptenoate; (2) cyclization of the latter with tosylmethyl isocyanide in DMSO to give a pyrrole derivative; (3) N-alkylation of the pyrrole using NaH and 1-naphthalenylmethyl chloride in DMF; and (4) cyclocondensation of the pyrrole sidechains with methylhydrazine. As inhibitors of human mixed lymphocyte reaction in vitro, the example compds. had IA<sub>50</sub> values of < 1 + 10<sup>-6</sup> M.

AN 1999:388188 CAPLUS <<LOGINID::20071212>>

DN 131:44836

TI Preparation of novel fused pyridazinones useful as immunosuppressants

IN Bantick, John; Cooper, Martin; Thorne, Philip; Perry, Matthew  
PA Astra Pharmaceuticals Ltd., UK; Astra Aktiebolag  
SO PCT Int. Appl., 94 pp.  
CODEN: PIXXD2

DT Patent  
LA English

FAN.CNT 2

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	TR 200001603	T2	20001023	TR 2000-1603	19981201
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	US 6770646	B2	20040803		
	US 2004162410	A1	20040819	US 2004-776245	20040212
PRAI	SE 1997-4542	A	19971205		
	SE 1998-1989	A	19980604		
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	SE 1996-556	A	19960215		
	WO 1996-SE1680	W	19961217		

=> s 18 not 14

L9 18 L8 NOT L4

=> d 19 1-18 ti abs bib hitstr

L9 ANSWER 1 OF 18 CAPLUS COPYRIGHT 2007 ACS on STN

TI Synthesis of 5-aryl-2-oxopyrrole derivatives as synthons for highly substituted pyrroles

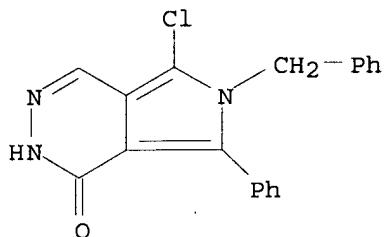
AB A small library of 2-oxo-5-(hetero)arylpyrroles was prepared starting from 2,3-dioxo-5-(hetero)arylpyrrolidines. The large synthetic possibilities of these 2-oxopyrroles were investigated. The 2-oxopyrroles offer a large number of possible derivatizations including reactions with electrophiles. The chloroformylation of 2-oxo-5-(hetero)arylpyrroles provides pyrrole carbaldehydes. Some pyrrole carbaldehydes were used to synthesize polycyclic compds. like pyrrolo[3,4-d]pyridazinones, a thienopyrrole, a pyrrolobenz[1,4]oxazepine, a pyrrolobenz[1,4]thiazepine, and a pyrrolobenz[1,4]diazepine. Hereby we showed through a short exploration that the oxopyrroles and analogs are interesting and versatile synthetic building blocks.

AN 2006:498781 CAPLUS <<LOGINID::20071212>>

DN 145:167033

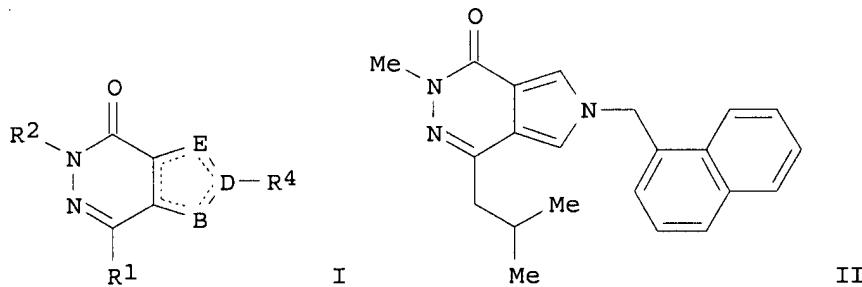
TI Synthesis of 5-aryl-2-oxopyrrole derivatives as synthons for highly

AU substituted pyrroles  
 Metten, Bert; Kostermans, Maarten; Van Baelen, Gitte; Smet, Mario; Dehaen, Wim  
 CS Department of Chemistry, Katholieke Universiteit Leuven, Louvain, B-3001, Belg.  
 SO Tetrahedron (2006), 62(25), 6018-6028  
 CODEN: TETRAB; ISSN: 0040-4020  
 PB Elsevier B.V.  
 DT Journal  
 LA English  
 OS CASREACT 145:167033  
 IT 901764-67-8P  
 RL: SPN (Synthetic preparation); PREP (Preparation)  
 (synthesis of library of 5-aryl-2-oxopyrrole derivs. from  
 2,3-dioxo-5-arylpyrrolidines and their use as synthons for highly  
 substituted pyrroles)  
 RN 901764-67-8 CAPLUS  
 CN 1H-Pyrrolo[3,4-d]pyridazin-1-one, 5-chloro-2,6-dihydro-7-phenyl-6-(phenylmethyl)- (CA INDEX NAME)



RE.CNT 31 THERE ARE 31 CITED REFERENCES AVAILABLE FOR THIS RECORD  
 ALL CITATIONS AVAILABLE IN THE RE FORMAT

L9 ANSWER 2 OF 18 CAPLUS COPYRIGHT 2007 ACS on STN  
 TI Preparation of novel fused pyridazinones useful as immunosuppressants  
 GI



AB The invention provides certain pyrrolo-, thieno-, furano- and  
 pyrazolo[3,4-d]pyridazinones of general formula I [B = CH, N, S, or O; D =  
 C or N; E = CR<sub>3</sub> or N; with various dependencies; R<sub>1</sub> = alkyl, alkoxy,  
 (di)(alkyl)amino, Ph, cycloalkyl, etc.; R<sub>2</sub> = Me, alkyl, alkoxyalkyl; R<sub>3</sub> =  
 H, (un)substituted carbamoyl, various derivs. of OH and SH; R<sub>4</sub> =  
 (un)substituted (hetero)aryl methyl, (hetero)aroyl,  
 (hetero)arylhydroxymethyl, acenaphthetyl, indanyl, or fluorenyl] and their

pharmaceutically acceptable salts or solvates. Also disclosed are processes for their preparation, pharmaceutical compns. containing them, a process

for preparing the pharmaceutical compns., and methods of treatment involving their use. In particular, their use in immunosuppression, and especially in therapy of reversible obstructive airways diseases, is claimed. For example, title compound II was prepared in 4 steps: (1) bromination of 4-methyl-2-pentanone and reaction with Ph3P:CHCO2Me to give (E)-Me 6-methyl-4-oxo-2-heptenoate; (2) cyclization of the latter with tosylmethyl isocyanide in DMSO to give a pyrrole derivative; (3) N-alkylation of the pyrrole using NaH and 1-naphthalenylmethyl chloride in DMF; and (4) cyclocondensation of the pyrrole sidechains with methylhydrazine. As inhibitors of human mixed lymphocyte reaction in vitro, the example compds. had IA50 values of < 1 + 10-6 M.

AN 1999:388188 CAPLUS <>LOGINID::20071212>>

DN 131:44836

TI Preparation of novel fused pyridazinones useful as immunosuppressants

IN Bantick, John; Cooper, Martin; Thorne, Philip; Perry, Matthew

PA Astra Pharmaceuticals Ltd., UK; Astra Aktiebolag

SO PCT Int. Appl., 94 pp.

CODEN: PIXXD2

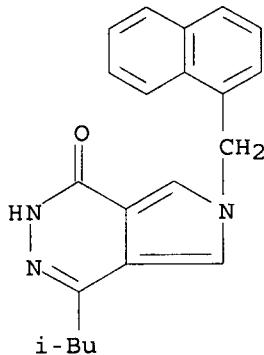
DT Patent

LA English

FAN.CNT 2

	PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI	WO 9929695	A1	19990617	WO 1998-SE2191	19981201
	W: AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, CA, CH, CN, CU, CZ, DE, DK, EE, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MD, MG, MK, MN, MW, MX, NO, NZ, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TR, TT, UA, UG, US, UZ, VN, YU, ZW				
	RW: GH, GM, KE, LS, MW, SD, SZ, UG, ZW, AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, BF, BJ, CF, CG, CI, CM, GA, GN, GW, ML, MR, NE, SN, TD, TG				
	CA 2312419	A1	19990617	CA 1998-2312419	19981201
	AU 9917916	A	19990628	AU 1999-17916	19981201
	EP 1036076	A1	20000920	EP 1998-962754	19981201
	EP 1036076	B1	20020904		
	R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO				
	BR 9813373	A	20001003	BR 1998-13373	19981201
	TR 200001603	T2	20001023	TR 2000-1603	19981201
	EE 200000318	A	20010815	EE 2000-318	19981201
	HU 2001000280	A2	20011028	HU 2001-280	19981201
	HU 2001000280	A3	20030328		
	JP 2001525413	T	20011211	JP 2000-524288	19981201
	NZ 504452	A	20020531	NZ 1998-504452	19981201
	AT 223413	T	20020915	AT 1998-962754	19981201
	US 6342601	B1	20020129	US 1999-214755	19990112
	NO 2000002788	A	20000801	NO 2000-2788	20000531
	US 2002099055	A1	20020725	US 2001-6244	20011210
	US 6770646	B2	20040803		
	US 2004162410	A1	20040819	US 2004-776245	20040212
PRAI	SE 1997-4542	A	19971205		
	SE 1998-1989	A	19980604		
	GB 1995-26273	A	19951221		
	SE 1996-556	A	19960215		
	WO 1996-SE1680	W	19961217		
	US 1997-776231	A1	19970131		
	WO 1998-SE2191	W	19981201		
	US 1999-214755	A3	19990112		
	US 1999-353644	A1	19990715		
	US 2000-708449	B1	20001109		

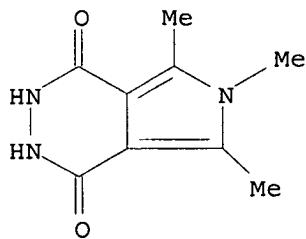
US 2002-74008 B1 20020214  
 OS MARPAT 131:44836  
 IT 227321-70-2P, 2,6-Dihydro-4-(2-methylpropyl)-6-(1-naphthalenylmethyl)-1H-pyrrolo[3,4-d]pyridazin-1-one  
 RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)  
 (intermediate; preparation of fused pyridazinones as immunosuppressants)  
 RN 227321-70-2 CAPLUS  
 CN 1H-Pyrrolo[3,4-d]pyridazin-1-one, 2,6-dihydro-4-(2-methylpropyl)-6-(1-naphthalenylmethyl)- (CA INDEX NAME)



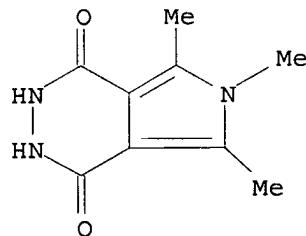
RE.CNT 6 THERE ARE 6 CITED REFERENCES AVAILABLE FOR THIS RECORD  
 ALL CITATIONS AVAILABLE IN THE RE FORMAT

L9 ANSWER 3 OF 18 CAPLUS COPYRIGHT 2007 ACS on STN  
 TI Investigation of the structure of and the properties of the potentially tautomeric 1,2,3,4-tetrahydro-5,7-dimethyl-6H-pyrrolo[3,4-d]pyridazine-1,4-diones in the gaseous and aqueous phases using the AM1 semi-empirical method  
 AB Potentially tautomeric 1,2,3,4-tetrahydro-5,7-dimethyl-6H-pyrrolo[3,4-d]pyridazine-1,4-diones and their fixed tautomeric forms have been studied in order to predict their tautomeric equilibrium consts. and pKa values using semi-empirical AM1 quantum-chemical calcns. at the SCF level in the gas phase and in aqueous solution. Hydroxy-oxo forms were found to be more stable than dioxo and dihydroxy forms. The results obtained from the tautomeric equilibrium and basicity calcns. are in good agreement with exptl. data.  
 AN 1998:451319 CAPLUS <>LOGINID::20071212>>  
 DN 129:175315  
 TI Investigation of the structure of and the properties of the potentially tautomeric 1,2,3,4-tetrahydro-5,7-dimethyl-6H-pyrrolo[3,4-d]pyridazine-1,4-diones in the gaseous and aqueous phases using the AM1 semi-empirical method  
 AU Guven, Alaattin; Oгretir, Cemil  
 CS Faculty of Science, Chemistry Department, Anadolu University, Eskiehir, Turk.  
 SO THEOCHEM (1998), 434, 7-28  
 CODEN: THEODJ; ISSN: 0166-1280  
 PB Elsevier Science B.V.  
 DT Journal  
 LA English  
 IT 96441-75-7 96441-82-6 211247-93-7  
 211247-94-8 211248-10-1 211389-39-8  
 211450-67-8  
 RL: PRP (Properties); RCT (Reactant); RACT (Reactant or reagent)  
 (structure of and properties of potentially tautomeric 1,2,3,4-tetrahydro-5,7-dimethyl-6H-pyrrolo[3,4-d]pyridazine-1,4-diones in gaseous and aqueous phases using AM1)

RN 96441-75-7 CAPLUS  
CN 1H-Pyrrolo[3,4-d]pyridazine-1,4(6H)-dione, 2,3-dihydro-5,6,7-trimethyl- (CA INDEX NAME)

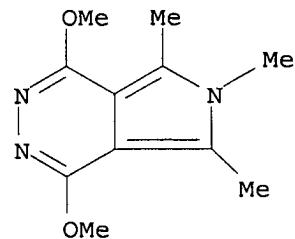


RN 96441-82-6 CAPLUS  
CN 1H-Pyrrolo[3,4-d]pyridazine-1,4(6H)-dione, 2,3-dihydro-5,6,7-trimethyl-, conjugate monoacid (9CI) (CA INDEX NAME)

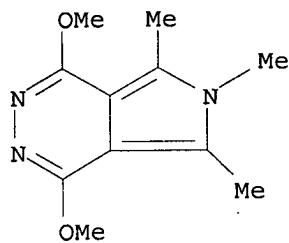


● H<sup>+</sup>

RN 211247-93-7 CAPLUS  
CN 6H-Pyrrolo[3,4-d]pyridazine, 1,4-dimethoxy-5,6,7-trimethyl- (CA INDEX NAME)



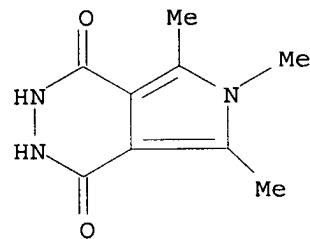
RN 211247-94-8 CAPLUS  
CN 6H-Pyrrolo[3,4-d]pyridazine, 1,4-dimethoxy-5,6,7-trimethyl-, conjugate monoacid (9CI) (CA INDEX NAME)



● H<sup>+</sup>

RN 211248-10-1 CAPLUS

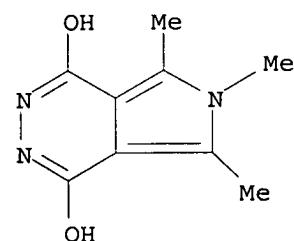
CN 1H-Pyrrolo[3,4-d]pyridazine-1,4(6H)-dione, 2,3-dihydro-5,6,7-trimethyl-, conjugate diacid (9CI) (CA INDEX NAME)



● 2 H<sup>+</sup>

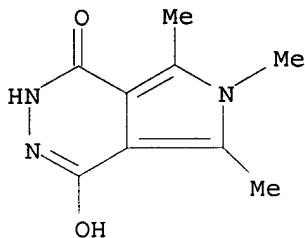
RN 211389-39-8 CAPLUS

CN 6H-Pyrrolo[3,4-d]pyridazine-1,4-diol, 5,6,7-trimethyl- (CA INDEX NAME)



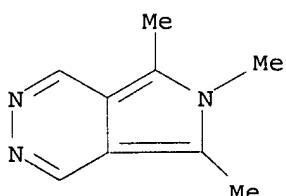
RN 211450-67-8 CAPLUS

CN 1H-Pyrrolo[3,4-d]pyridazin-1-one, 2,6-dihydro-4-hydroxy-5,6,7-trimethyl- (CA INDEX NAME)

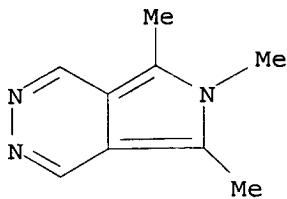


RE.CNT 11 THERE ARE 11 CITED REFERENCES AVAILABLE FOR THIS RECORD  
ALL CITATIONS AVAILABLE IN THE RE FORMAT

L9 ANSWER 4 OF 18 CAPLUS COPYRIGHT 2007 ACS on STN  
 TI Investigation of the structure and properties of the potentially tautomeric 5,7-dimethyl-6H-pyrrolo[3,4-d]pyridazines in the gas and aqueous phases using the AM1 and PM3/COSMO solvation method  
 AB The potentially tautomeric 5,7-dimethyl-6H-pyrrolo[3,4-d]pyridazines, 2H and 6H, and their fixed tautomeric forms were studied in order to predict the most stable form by the restricted Hartree-Foch approach using semiempirical PM3 and AM1 quantum chemical calcns. at the SCF level in the gas and aqueous phases. Both methods predicted that the 6H form is more stable than the other forms in both gas and aqueous phases. The results obtained were found to be in agreement with the exptl. data. Monoprotonated forms of 5,7-dimethyl-6H-pyrrolo[3,4-d]pyridazines were also examined. Proton affinity calcns. predicted that the first protonations take place on the N6 atom in the 2H form and on the N2 atom in the 6H form, resulting in a common cation.  
 AN 1998:220258 CAPLUS <>LOGINID::20071212>>  
 DN 128:321258  
 TI Investigation of the structure and properties of the potentially tautomeric 5,7-dimethyl-6H-pyrrolo[3,4-d]pyridazines in the gas and aqueous phases using the AM1 and PM3/COSMO solvation method  
 AU Guven, Alaattin; Ogretir, Cemil  
 CS Fac. Sci., Chem. Dep., Anadolu Univ., Eskisehir, Turk.  
 SO THEOCHEM (1998), 430, 85-95  
 CODEN: THEODJ; ISSN: 0166-1280  
 PB Elsevier Science B.V.  
 DT Journal  
 LA English  
 IT 30476-58-5 206860-75-5 206860-78-8  
 RL: PRP (Properties)  
 (AM1 and PM3/COSMO solvation method in study of tautomeric nature of 5,7-dimethyl-6H-pyrrolo[3,4-d]pyridazines in gas and aqueous phases)  
 RN 30476-58-5 CAPLUS  
 CN 6H-Pyrrolo[3,4-d]pyridazine, 5,6,7-trimethyl- (8CI, 9CI) (CA INDEX NAME)

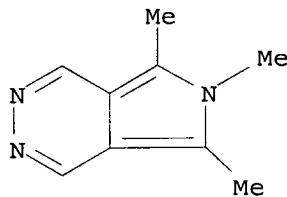


RN 206860-75-5 CAPLUS  
 CN 6H-Pyrrolo[3,4-d]pyridazine, 5,6,7-trimethyl-, conjugate monoacid (9CI)  
 (CA INDEX NAME)



● H<sup>+</sup>

RN 206860-78-8 CAPLUS  
CN 6H-Pyrrolo[3,4-d]pyridazine, 5,6,7-trimethyl-, conjugate diacid (9CI) (CA  
INDEX NAME)

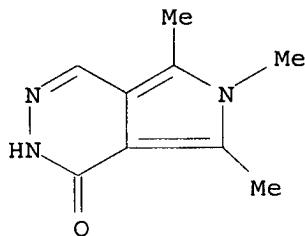


● 2 H<sup>+</sup>

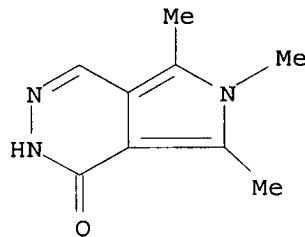
RE.CNT 11 THERE ARE 11 CITED REFERENCES AVAILABLE FOR THIS RECORD  
ALL CITATIONS AVAILABLE IN THE RE FORMAT

L9 ANSWER 5 OF 18 CAPLUS COPYRIGHT 2007 ACS on STN  
TI Investigation of the structure and the properties of the potentially  
tautomeric 1,2-dihydro-5,7-dimethyl-6H-pyrrolo[3,4-d]pyridazine-1-ones in  
the gas and aqueous phases using semiempirical methods  
AB Potentially tautomeric 1,2-dihydro-5,7-dimethyl-6H-pyrrolo[3,4-  
d]pyridazine-1-ones and their fixed tautomeric forms have been studied, in  
order to predict their tautomeric equilibrium consts. and pKa values, using  
semiempirical PM3, AM1 quantum-chemical calcns. at the SCF level in the gas  
phase and in aqueous solution. The effect of alkylation on the pKa value was  
also  
investigated. In both the gas phase and in aqueous solution, oxo forms have  
been  
found to be more stable than hydroxy and zwitterionic structures. The  
results obtained from the tautomeric equilibrium and acidity calcns. are in  
good agreement with exptl. data.  
AN 1998:199391 CAPLUS <>LOGINID::20071212>>  
DN 129:4401  
TI Investigation of the structure and the properties of the potentially  
tautomeric 1,2-dihydro-5,7-dimethyl-6H-pyrrolo[3,4-d]pyridazine-1-ones in  
the gas and aqueous phases using semiempirical methods  
AU Guven, Alaatin; Ogretir, Cemil  
CS Fac. Sci., Chem. Dep., Anadolu Univ., Eskisehir, Turk.  
SO THEOCHEM (1998), 427, 65-77  
CODEN: THEODJ; ISSN: 0166-1280  
PB Elsevier Science B.V.

DT Journal  
LA English  
IT 90817-87-1 96441-64-4 207286-20-2  
207286-21-3 207286-22-4 207286-23-5  
207286-24-6 207286-25-7 207286-26-8  
207355-02-0 207355-03-1 207355-04-2  
RL: PEP (Physical, engineering or chemical process); PRP (Properties); RCT  
(Reactant); PROC (Process); RACT (Reactant or reagent)  
(structure and properties of potentially tautomeric  
1,2-dihydro-5,7-dimethyl-6H-pyrrolo[3,4-d]pyridazine-1-ones in gas and  
aqueous phases using semiempirical methods)  
RN 90817-87-1 CAPLUS  
CN 1H-Pyrrolo[3,4-d]pyridazin-1-one, 2,6-dihydro-5,6,7-trimethyl- (CA INDEX  
NAME)

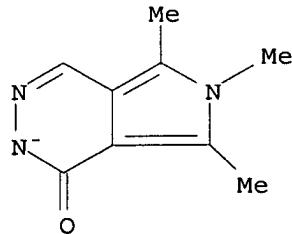


RN 96441-64-4 CAPLUS  
CN 1H-Pyrrolo[3,4-d]pyridazin-1-one, 2,6-dihydro-5,6,7-trimethyl-, conjugate  
monoacid (9CI) (CA INDEX NAME)

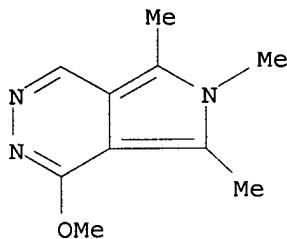


● H<sup>+</sup>

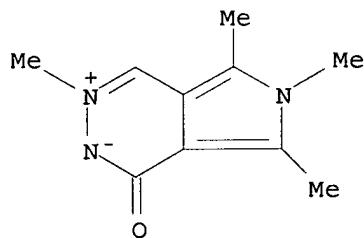
RN 207286-20-2 CAPLUS  
CN 1H-Pyrrolo[3,4-d]pyridazin-1-one, 2,6-dihydro-5,6,7-trimethyl-, ion(1-)  
(CA INDEX NAME)



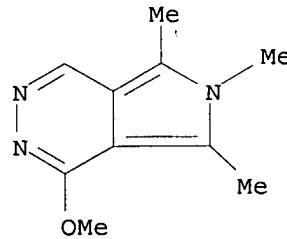
RN 207286-21-3 CAPLUS  
CN 6H-Pyrrolo[3,4-d]pyridazine, 1-methoxy-5,6,7-trimethyl- (CA INDEX NAME)



RN 207286-22-4 CAPLUS  
CN 1H-Pyrrolo[3,4-d]pyridazinium, 2,6-dihydro-3,5,6,7-tetramethyl-1-oxo-,  
inner salt (CA INDEX NAME)

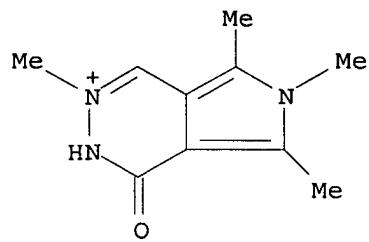


RN 207286-23-5 CAPLUS  
CN 6H-Pyrrolo[3,4-d]pyridazine, 1-methoxy-5,6,7-trimethyl-, conjugate  
monoacid (9CI) (CA INDEX NAME)

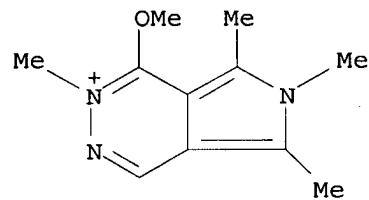


● H<sup>+</sup>

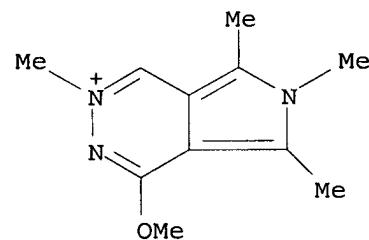
RN 207286-24-6 CAPLUS  
CN 1H-Pyrrolo[3,4-d]pyridazinium, 2,6-dihydro-3,5,6,7-tetramethyl-1-oxo- (CA  
INDEX NAME)



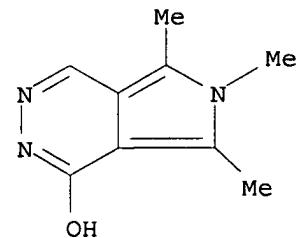
RN 207286-25-7 CAPLUS  
CN 6H-Pyrrolo[3,4-d]pyridazinium, 1-methoxy-2,5,6,7-tetramethyl- (CA INDEX NAME)



RN 207286-26-8 CAPLUS  
CN 6H-Pyrrolo[3,4-d]pyridazinium, 4-methoxy-2,5,6,7-tetramethyl- (CA INDEX NAME)

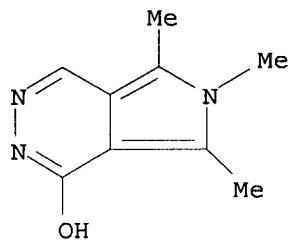


RN 207355-02-0 CAPLUS  
CN 6H-Pyrrolo[3,4-d]pyridazin-1-ol, 5,6,7-trimethyl-, conjugate monoacid (9CI) (CA INDEX NAME)



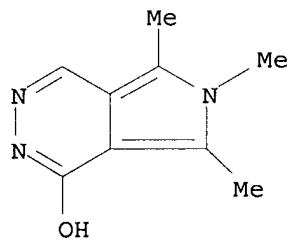
● H<sup>+</sup>

RN 207355-03-1 CAPLUS  
CN 6H-Pyrrolo[3,4-d]pyridazin-1-ol, 5,6,7-trimethyl-, conjugate diacid (9CI)  
(CA INDEX NAME)



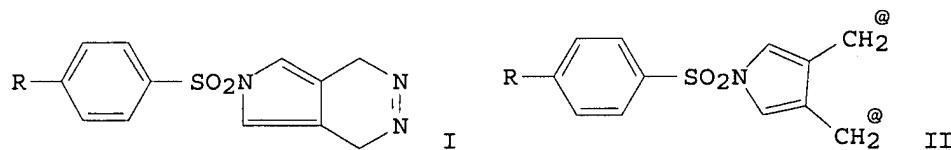
● 2 H<sup>+</sup>

RN 207355-04-2 CAPLUS  
CN 6H-Pyrrolo[3,4-d]pyridazin-1-ol, 5,6,7-trimethyl- (CA INDEX NAME)



RE.CNT 21 THERE ARE 21 CITED REFERENCES AVAILABLE FOR THIS RECORD  
ALL CITATIONS AVAILABLE IN THE RE FORMAT

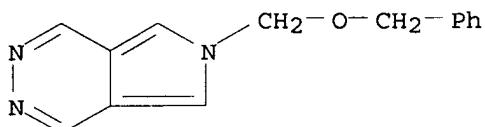
L9 ANSWER 6 OF 18 CAPLUS COPYRIGHT 2007 ACS on STN  
TI Long-lived spin isomerism of singlet and triplet states of  
N-arenesulfonyl-3,4-dimethylenepyrroles  
GI



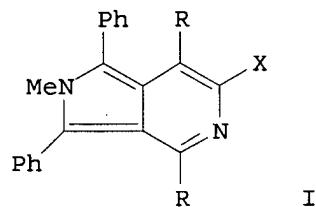
AB A theor. prediction that attachment of an electron-withdrawing group to the ring nitrogen of a 3,4-dimethylenepyrrole biradical should selectively stabilize the triplet state is tested by generation of matrix-immobilized transient species in the irradiation of 1,4-dihydro-6-arenesulfonylpyrrolo[3,4-d]pyridazine precursors (I; R = Me, Br) at 265 nm. ESR spectra of triplet species assigned to the corresponding dimethylenepyrroles (II) are observed in both cases. The zero-field splitting parameter D is 0.023 cm<sup>-1</sup> in both cases, essentially the same as those reported in the literature for

tetramethyleneethane derivs. Irradiation of the precursors at 370 nm gives rise in both cases to the corresponding singlets, blue ( $\lambda_{\text{max}}$  593 and 600 nm, resp.), ESR-silent substances. The spin isomers do not interconvert over a period of days.

AN 1994:133629 CAPLUS <<LOGINID::20071212>>  
DN 120:133629  
TI Long-lived spin isomerism of singlet and triplet states of N-arenesulfonyl-3,4-dimethylenepyrroles  
AU Bush, Linda C.; Heath, Richard B.; Berson, Jerome A.  
CS Dep. Chem., Yale Univ., New Haven, CT, 06511, USA  
SO Journal of the American Chemical Society (1993), 115(21), 9830-1  
CODEN: JACSAT; ISSN: 0002-7863  
DT Journal  
LA English  
IT 152940-60-8P  
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)  
(preparation and reduction of)  
RN 152940-60-8 CAPLUS  
CN 6H-Pyrrolo[3,4-d]pyridazine, 6-[(phenylmethoxy)methyl]- (CA INDEX NAME)



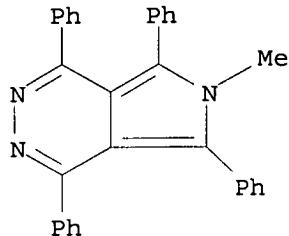
L9 ANSWER 7 OF 18 CAPLUS COPYRIGHT 2007 ACS on STN  
TI Substituent effects on the spectra of fluorescent aryl-substituted N-methylpyrrolo[3,4-c]pyridines  
GI



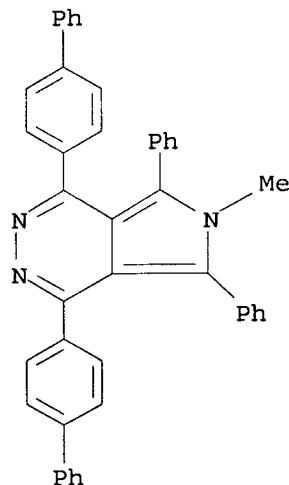
AB Introduction of an alkoxy group into the Ph ring at the 4 and 7 positions of I (R = aryl; X = CN, CONH<sub>2</sub>, CO<sub>2</sub>H) had little effect on the absorption and emission spectra of the title dyes, while introduction of a Br group caused a red shift in the spectrum of I (X = CN). I (X = CN, CO<sub>2</sub>Et, H) were strongly fluorescent, while the fluorescence of I (X = CONH<sub>2</sub>) was weak; I (X = CONHNH<sub>2</sub>, CO<sub>2</sub>H) were also weakly fluorescent with a large Stokes shift (.apprx.150 nm). Related pyridazines were not fluorescent.

AN 1993:82819 CAPLUS <<LOGINID::20071212>>  
DN 118:82819  
TI Substituent effects on the spectra of fluorescent aryl-substituted N-methylpyrrolo[3,4-c]pyridines  
AU Mataka, Shuntaro; Tashiro, Masashi; Misumi, Osamu; Lin, Wei Hua; Takahashi, Kazufumi; Torii, Akiyoshi  
CS Inst. Adv. Mater. Study, Kyushu Univ., Kasuga, 816, Japan  
SO Dyes and Pigments (1992), 20(2), 83-96  
CODEN: DYPIDX; ISSN: 0143-7208

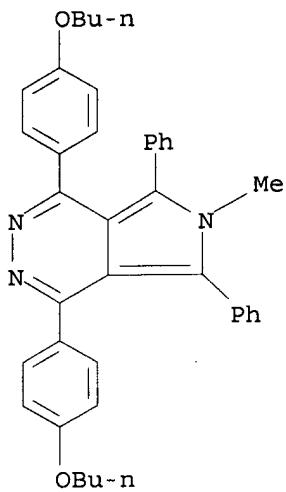
DT Journal  
LA English  
IT 145551-53-7P 145551-54-8P 145551-55-9P  
RL: PRP (Properties); SPN (Synthetic preparation); PREP (Preparation)  
(preparation and fluorescence of, substituent effect in relation to)  
RN 145551-53-7 CAPLUS  
CN 6H-Pyrrolo[3,4-d]pyridazine, 6-methyl-1,4,5,7-tetraphenyl- (CA INDEX  
NAME)



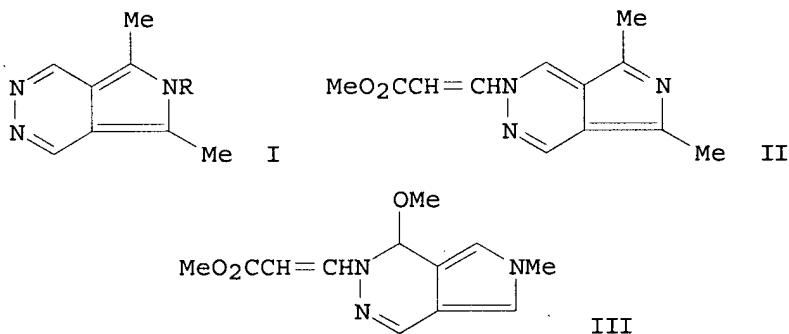
RN 145551-54-8 CAPLUS  
CN 6H-Pyrrolo[3,4-d]pyridazine, 1,4-bis([1,1'-biphenyl]-4-yl)-6-methyl-5,7-  
diphenyl- (CA INDEX NAME)



RN 145551-55-9 CAPLUS  
CN 6H-Pyrrolo[3,4-d]pyridazine, 1,4-bis(4-butoxyphenyl)-6-methyl-5,7-diphenyl-  
(CA INDEX NAME)

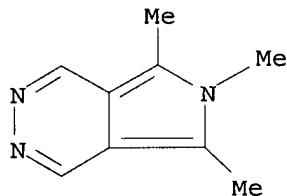


L9 ANSWER 8 OF 18 CAPLUS COPYRIGHT 2007 ACS on STN  
 TI Pyrrole studies. Part 39. The disparate reactivity of  
 5,7-dimethyl-6H-pyrrolo[3,4-d]pyridazines with acetylenic esters and with  
 azodicarboxylic esters  
 GI

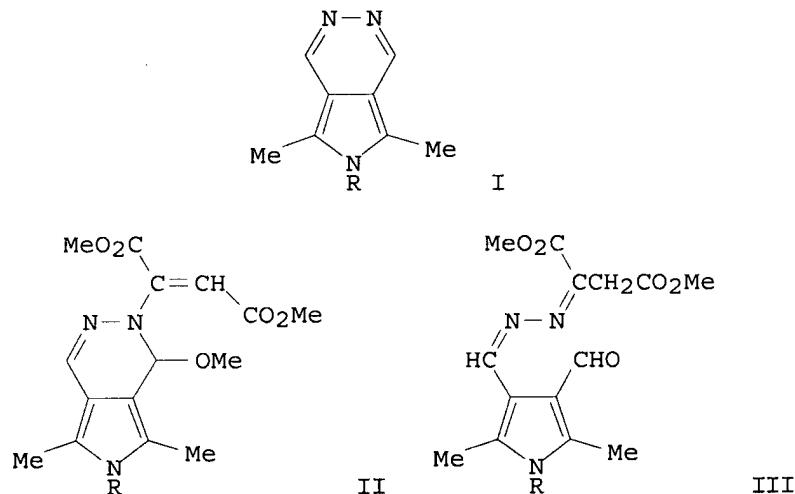


AB Reaction of MeO<sub>2</sub>CC.tplbond.CH with the title pyrrolopyridazines I (R = H, Me) in MeOH gave adducts II and III, resp., but no ring opened products. In contrast, EtO<sub>2</sub>CN:NCO<sub>2</sub>Et underwent reaction with I (R = H) at the electron-rich 5-membered ring.  
 AN 1988:510358 CAPLUS <<LOGINID::20071212>>  
 DN 109:110358  
 TI Pyrrole studies. Part 39. The disparate reactivity of  
 5,7-dimethyl-6H-pyrrolo[3,4-d]pyridazines with acetylenic esters and with  
 azodicarboxylic esters  
 AU Fuentes Rodriguez, Fernanda; Sepulveda-Arques, Jose; Jones, R. Alan  
 CS Fac. Farm., Univ. Valencia, Valencia, 46010, Spain  
 SO Journal of Chemical Research, Synopses (1987), (11), 356  
 CODEN: JRPSDC; ISSN: 0308-2342  
 DT Journal  
 LA English  
 OS CASREACT 109:110358  
 IT 30476-58-5  
 RL: RCT (Reactant); RACT (Reactant or reagent)  
 (addition reaction of, with Me propiolate)  
 RN 30476-58-5 CAPLUS

CN 6H-Pyrrolo[3,4-d]pyridazine, 5,6,7-trimethyl- (8CI, 9CI) (CA INDEX NAME)



L9 ANSWER 9 OF 18 CAPLUS COPYRIGHT 2007 ACS on STN  
TI Pyrrole studies. Part 32. A novel ring-cleavage reaction of the pyridazine ring during the reaction of 6H-pyrrolo[3,4-d]pyridazines with dimethyl acetylenedicarboxylate  
GI



AB Treatment of pyrrolopyridazines I (R = Me, H, Ph) with (MeO2CC.tplbond.)2 in MeOH at -70° gave the corresponding esters II (R as before), which were unstable in the presence of H2O and underwent ring cleavage to the corresponding pyrroles III. The structure of III (R = H) was confirmed by x-ray anal.

AN 1985:471267 CAPLUS <>LOGINID::20071212>>

DN 103:71267

TI Pyrrole studies. Part 32. A novel ring-cleavage reaction of the pyridazine ring during the reaction of 6H-pyrrolo[3,4-d]pyridazines with dimethyl acetylenedicarboxylate

AU Hernandez de la Figuera Gomez, Teresa; Sepulveda Arques, Jose; Jones, R. Alan; Dawes, Helen M.; Hursthouse, Michael B.

CS Dep. Quim. Org., Univ. Valencia, Valencia, Spain

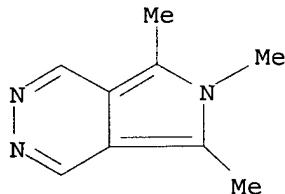
SO Journal of the Chemical Society, Perkin Transactions 1: Organic and Bio-Organic Chemistry (1972-1999) (1985), (4), 899-902  
CODEN: JCPRB4; ISSN: 0300-922X

DT Journal

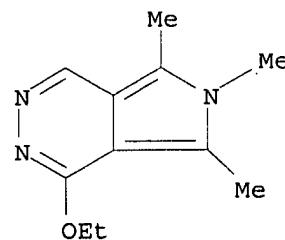
LA English

OS CASREACT 103:71267

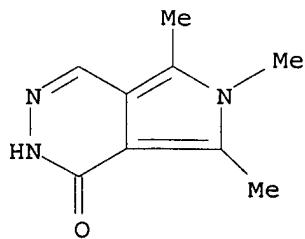
IT 30476-58-5  
RL: RCT (Reactant); RACT (Reactant or reagent)  
(reaction of, with di-Me acetylenedicarboxylate)  
RN 30476-58-5 CAPLUS  
CN 6H-Pyrrolo[3,4-d]pyridazine, 5,6,7-trimethyl- (8CI, 9CI) (CA INDEX NAME)



L9 ANSWER 10 OF 18 CAPLUS COPYRIGHT 2007 ACS on STN  
TI Pyrrole studies: 31. The structures of potentially tautomeric 1,2-dihydro-6H-pyrrolo[3,4-d]pyridazin-1-ones and 1,2,3,4-tetrahydro-6H-pyrrolo[3,4-d]pyridazine-1,4-diones  
AB 1,2-Dihydro-6H-pyrrolo[3,4-d]pyridazin-1-ones exist predominantly as such in equilibrium with the 1-hydroxypyridazine form, whereas 1,2,3,4-tetrahydro-6H-pyrrolo[3,4-d]pyridazine-1,4-diones in equilibrium with the monohydroxy-oxo tautomeric forms are preferred by a factor of only .apprx.100:1. It was not possible to determine the position of equilibrium between the 1-hydroxy-6H-pyrrolo[3,4-d]pyridazin-4-one and the 1,4-dihydroxy-6H-pyrrolo[3,4-d]pyridazine structures.  
AN 1985:422083 CAPLUS <<LOGINID::20071212>>  
DN 103:22083  
TI Pyrrole studies: 31. The structures of potentially tautomeric 1,2-dihydro-6H-pyrrolo[3,4-d]pyridazin-1-ones and 1,2,3,4-tetrahydro-6H-pyrrolo[3,4-d]pyridazine-1,4-diones  
AU Inel, Sermin; Jones, R. Alan; Ogretir, Cemil  
CS Sch. Chem. Sci., Univ. East Anglia, Norwich, NR4 7TJ, UK  
SO Tetrahedron (1984), 40(20), 3979-86  
CODEN: TETRAB; ISSN: 0040-4020  
DT Journal  
LA English  
OS CASREACT 103:22083  
IT 96441-62-2 96441-64-4 96441-67-7  
96441-69-9 96441-72-4 96441-73-5  
96441-80-4 96441-82-6 96441-86-0  
96441-88-2  
RL: PRP (Properties)  
(UV spectrum of)  
RN 96441-62-2 CAPLUS  
CN 6H-Pyrrolo[3,4-d]pyridazine, 1-ethoxy-5,6,7-trimethyl- (CA INDEX NAME)

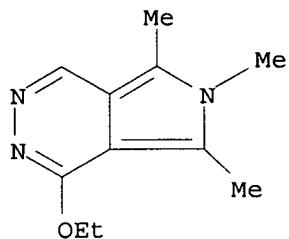


RN 96441-64-4 CAPLUS  
CN 1H-Pyrrolo[3,4-d]pyridazin-1-one, 2,6-dihydro-5,6,7-trimethyl-, conjugate monoacid (9CI) (CA INDEX NAME)



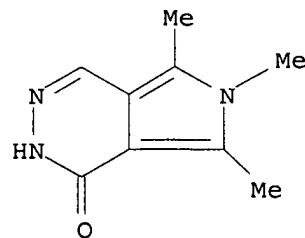
● H<sup>+</sup>

RN 96441-67-7 CAPLUS  
CN 6H-Pyrrolo[3,4-d]pyridazine, 1-ethoxy-5,6,7-trimethyl-, conjugate monoacid (9CI) (CA INDEX NAME)



● H<sup>+</sup>

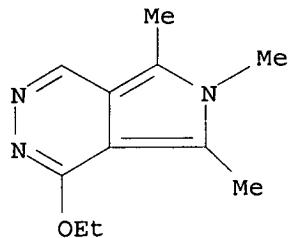
RN 96441-69-9 CAPLUS  
CN 1H-Pyrrolo[3,4-d]pyridazin-1-one, 2,6-dihydro-5,6,7-trimethyl-, conjugate diacid (9CI) (CA INDEX NAME)



● 2 H<sup>+</sup>

RN 96441-72-4 CAPLUS

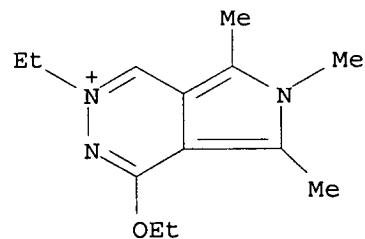
CN 6H-Pyrrolo[3,4-d]pyridazine, 1-ethoxy-5,6,7-trimethyl-, conjugate diacid (9CI) (CA INDEX NAME)



● 2 H<sup>+</sup>

RN 96441-73-5 CAPLUS

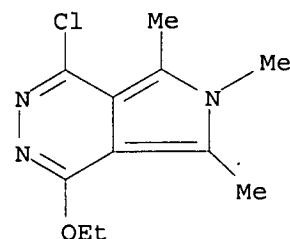
CN 6H-Pyrrolo[3,4-d]pyridazinium, 4-ethoxy-2-ethyl-5,6,7-trimethyl-, conjugate monoacid (9CI) (CA INDEX NAME)



● H<sup>+</sup>

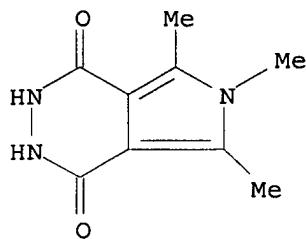
RN 96441-80-4 CAPLUS

CN 6H-Pyrrolo[3,4-d]pyridazine, 1-chloro-4-ethoxy-5,6,7-trimethyl- (CA INDEX NAME)



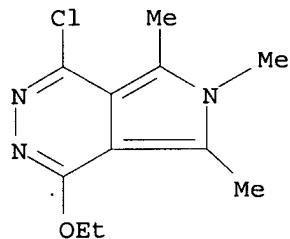
RN 96441-82-6 CAPLUS

CN 1H-Pyrrolo[3,4-d]pyridazine-1,4(6H)-dione, 2,3-dihydro-5,6,7-trimethyl-, conjugate monoacid (9CI) (CA INDEX NAME)



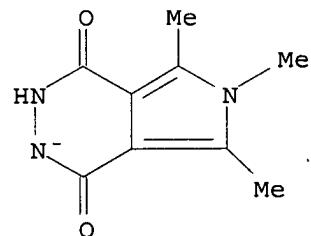
● H<sup>+</sup>

RN 96441-86-0 CAPLUS  
CN 6H-Pyrrolo[3,4-d]pyridazine, 1-chloro-4-ethoxy-5,6,7-trimethyl-, conjugate monoacid (9CI) (CA INDEX NAME)

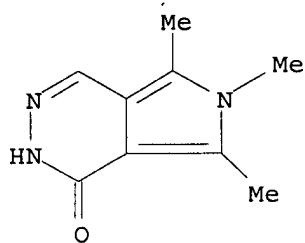


● H<sup>+</sup>

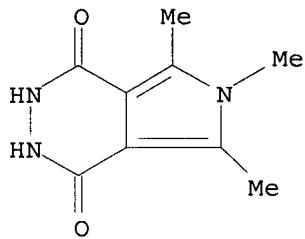
RN 96441-88-2 CAPLUS  
CN 1H-Pyrrolo[3,4-d]pyridazine-1,4(6H)-dione, 2,3-dihydro-5,6,7-trimethyl-, ion(1-) (CA INDEX NAME)



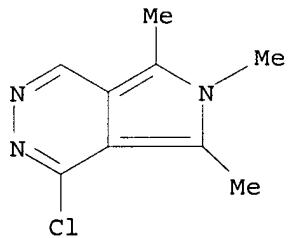
IT 90817-87-1 96441-75-7  
RL: PRP (Properties)  
(UV spectrum of, absence of tautomerism in relation to)  
RN 90817-87-1 CAPLUS  
CN 1H-Pyrrolo[3,4-d]pyridazin-1-one, 2,6-dihydro-5,6,7-trimethyl- (CA INDEX NAME)



RN 96441-75-7 CAPLUS  
 CN 1H-Pyrrolo[3,4-d]pyridazine-1,4(6H)-dione, 2,3-dihydro-5,6,7-trimethyl-  
 (CA INDEX NAME)

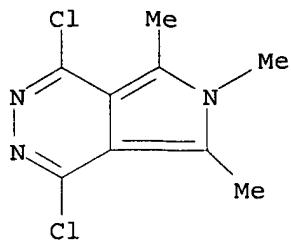


IT 96441-91-7P  
 RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT  
 (Reactant or reagent)  
 (preparation and reaction with sodium methoxide)  
 RN 96441-91-7 CAPLUS  
 CN 6H-Pyrrolo[3,4-d]pyridazine, 1-chloro-5,6,7-trimethyl-, monohydrochloride  
 (9CI) (CA INDEX NAME)



● HCl

IT 96441-92-8P 96452-45-8P 96452-47-0P  
 RL: SPN (Synthetic preparation); PREP (Preparation)  
 (preparation of)  
 RN 96441-92-8 CAPLUS  
 CN 6H-Pyrrolo[3,4-d]pyridazine, 1,4-dichloro-5,6,7-trimethyl- (CA INDEX  
 NAME)



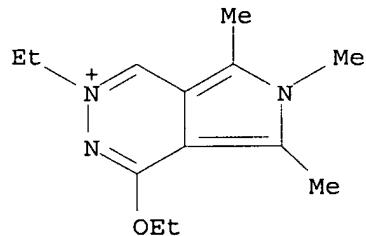
RN 96452-45-8 CAPLUS

CN 6H-Pyrrolo[3,4-d]pyridazinium, 4-ethoxy-2-ethyl-5,6,7-trimethyl-, tetrafluoroborate(1-) (9CI) (CA INDEX NAME)

CM 1

CRN 96452-44-7

CMF C13 H20 N3 O

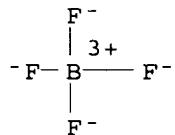


CM 2

CRN 14874-70-5

CMF B F4

CCI CCS



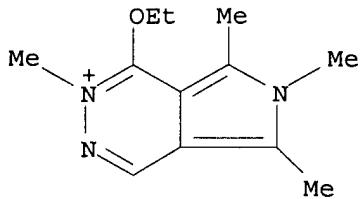
RN 96452-47-0 CAPLUS

CN 6H-Pyrrolo[3,4-d]pyridazinium, 1-ethoxy-2,5,6,7-tetramethyl-, tetrafluoroborate(1-) (9CI) (CA INDEX NAME)

CM 1

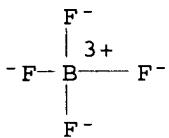
CRN 96452-46-9

CMF C12 H18 N3 O



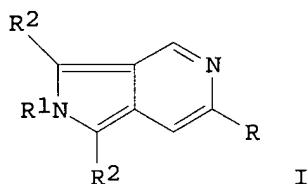
CM 2

CRN 14874-70-5  
 CMF B F4  
 CCI CCS



L9 ANSWER 11 OF 18 CAPLUS COPYRIGHT 2007 ACS on STN  
 TI Structure and reactivity of iso-fused heterocyclic systems with  $4n \pi$  and  $(4n + 2) \pi$  electrons. 8. Cyclizing condensation of 1H-pyrrole-3,4-dicarbaldehydes with 1,2-bifunctional compounds. A general and simple preparation method for 2H-pyrrolo[3,4-c]pyridines and 6H-pyrrolo[3,4-d]pyridazines

GI



AB 2H-Pyrrolo[3,4-c]pyridines I (R = CO2Me, CO2Et, cyano; R1 = H, Me, CMe3, CH2Ph; R2 = H, Me) are easily and efficiently accessible via reaction of 1H-pyrrole-3,4-dicarbaldehydes with H2NCH2R.HCl. Under the influence of Et2NH the cyclocondensation occurs in an uniform fashion and in 55-99% yields. In a similar manner 1H-pyrrole-3,4-dicarbaldehydes react with N2H4; two-fold elimination of H2O leads to 6H-pyrrolo[3,4-d]pyridazines. The bicyclic hetarenes are stabilized compared with 2H-isooindoles by addnl. heteroatoms in the 6-membered ring and acceptor groups at the 6-position.

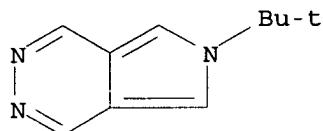
AN 1985:45802 CAPLUS <<LOGINID::20071212>>

DN 102:45802

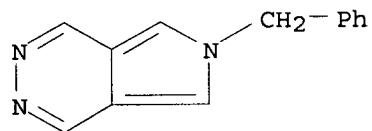
TI Structure and reactivity of iso-fused heterocyclic systems with  $4n \pi$  and  $(4n + 2) \pi$  electrons. 8. Cyclizing condensation of 1H-pyrrole-3,4-dicarbaldehydes with 1,2-bifunctional compounds. A general and simple preparation method for 2H-pyrrolo[3,4-c]pyridines and 6H-pyrrolo[3,4-d]pyridazines

AU Kreher, Richard P.; Pfister, Juergen

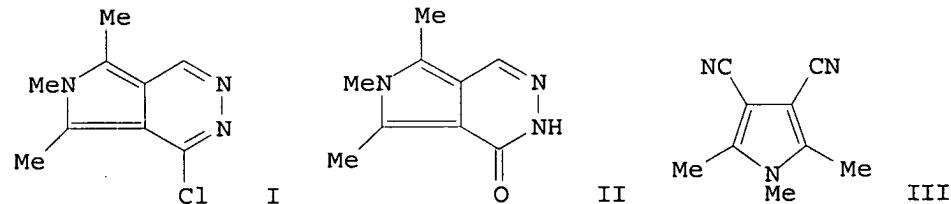
CS Abt. Chem., Univ. Dortmund, Dortmund, D-4600/50, Fed. Rep. Ger.  
 SO Chemiker-Zeitung (1984), 108(9), 275-7  
 CODEN: CMKZAT; ISSN: 0009-2894  
 DT Journal  
 LA German  
 OS CASREACT 102:45802  
 IT 94169-85-4P 94169-86-5P  
 RL: SPN (Synthetic preparation); PREP (Preparation)  
 (preparation of)  
 RN 94169-85-4 CAPLUS  
 CN 6H-Pyrrolo[3,4-d]pyridazine, 6-(1,1-dimethylethyl)- (CA INDEX NAME)



RN 94169-86-5 CAPLUS  
 CN 6H-Pyrrolo[3,4-d]pyridazine, 6-(phenylmethyl)- (CA INDEX NAME)

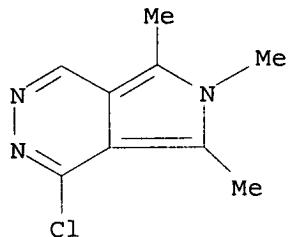


L9 ANSWER 12 OF 18 CAPLUS COPYRIGHT 2007 ACS on STN  
 TI Pyrrole studies. XXIX. An unusual pyridazine ring-opening reaction  
 GI

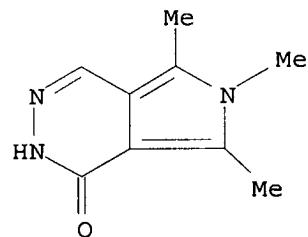


AB Treating 1-chloro-5,6,7-trimethylpyrrolo[3,4-d]pyridazine (I) with aqueous or  
 alc. NaOH, NaOEt, or NaOPh gave .apprx.60% pyridazinone II. Treating I  
 with NaOMe in DMF gave 42% dicyanopyrrole III and 40% II; NaOEt in DMF  
 gave 19% III.  
 AN 1984:423418 CAPLUS <>LOGINID::20071212>>  
 DN 101:23418  
 TI Pyrrole studies. XXIX. An unusual pyridazine ring-opening reaction  
 AU Jones, R. Alan; Inel, Sermin  
 CS Sch. Chem. Sci., Univ. East Anglia, Norwich, NR4 7TJ, UK  
 SO Chemistry & Industry (London, United Kingdom) (1984), (7), 270-1  
 CODEN: CHINAG; ISSN: 0009-3068  
 DT Journal  
 LA English  
 OS CASREACT 101:23418

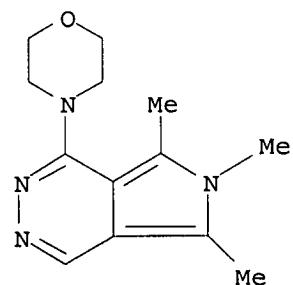
IT 90817-88-2  
RL: RCT (Reactant); RACT (Reactant or reagent)  
(base-catalyzed ring cleavage of)  
RN 90817-88-2 CAPLUS  
CN 6H-Pyrrolo[3,4-d]pyridazine, 1-chloro-5,6,7-trimethyl- (CA INDEX NAME)



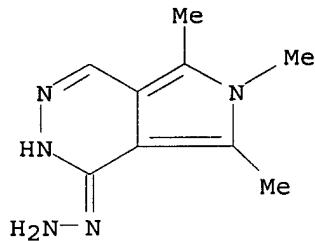
IT 90817-87-1P  
RL: FORM (Formation, nonpreparative); PREP (Preparation)  
(formation of, in ring cleavage of chlorotrimethylpyrrolopyridazine)  
RN 90817-87-1 CAPLUS  
CN 1H-Pyrrolo[3,4-d]pyridazin-1-one, 2,6-dihydro-5,6,7-trimethyl- (CA INDEX NAME)



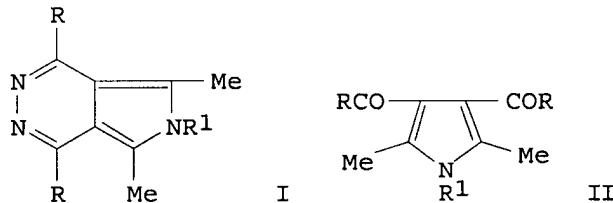
IT 90817-90-6P 90817-91-7P  
RL: SPN (Synthetic preparation); PREP (Preparation)  
(preparation of)  
RN 90817-90-6 CAPLUS  
CN 6H-Pyrrolo[3,4-d]pyridazine, 5,6,7-trimethyl-1-(4-morpholinyl)- (CA INDEX NAME)



RN 90817-91-7 CAPLUS  
CN 1H-Pyrrolo[3,4-d]pyridazin-1-one, 2,6-dihydro-5,6,7-trimethyl-, hydrazone (9CI) (CA INDEX NAME)



L9 ANSWER 13 OF 18 CAPLUS COPYRIGHT 2007 ACS on STN  
 TI Pyrrole studies. XXV. Structure of potentially tautomeric  
 pyrrolo[3,4-d]pyridazines  
 GI



AB Pyrrolopyridazines I (R = H, Me, R1 = H) were prepared by treating the pyrroles II with N2H4. II (R = R1 = H) was obtained by formylating 2,5-dimethylpyrrole and II (R = Me, R1 = H) from Ac2CHCHAc2 and NH4OAc. Methylation gave II (R = H, Me, R1 = Me) which were treated with N2H4 to give I (R = H, Me, R1 = Me). Quaternized derivs. were obtained with MeNHNH2 and MeNHNHMe or by quaternizing I. Electron spectra and basicity measurement showed that I exist in a 6H-form in accordance with MO calcns. of the relative resonance energies of the possible tautomers. Protonation occurs at the heteroatoms and at C-5.

AN 1981:569111 CAPLUS <<LOGINID::20071212>>

DN 95:169111

OREF 95:28269a,28272a

TI Pyrrole studies. XXV. Structure of potentially tautomeric  
 pyrrolo[3,4-d]pyridazines

AU Acar, Fatma; Badesha, Santokh Singh; Flitsch, Wilhelm; Gozogul, Reyhan;  
 Inel, Oguz; Inel, Sermin; Jones, R. Alan; Ogretir, Cemil; Rustidge, David  
 C.

CS Kim. Lab., Devlet Mimarlik Muhendislik Akad., Eskisehir, Turk.

SO Chimica Acta Turcica (1981), 9(1), 225-37

CODEN: CATUA9; ISSN: 0379-5896

DT Journal

LA English

OS CASREACT 95:169111

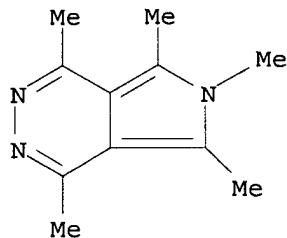
IT 79398-46-2P

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT  
 (Reactant or reagent)

(preparation and quaternization of)

RN 79398-46-2 CAPLUS

CN 6H-Pyrrolo[3,4-d]pyridazine, 1,4,5,6,7-pentamethyl- (CA INDEX NAME)



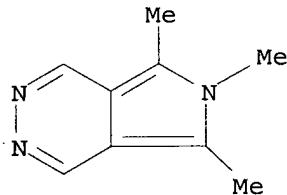
IT 30476-58-5P 79398-41-7P 79398-43-9P

79398-49-5P

RL: SPN (Synthetic preparation); PREP (Preparation)  
(preparation of)

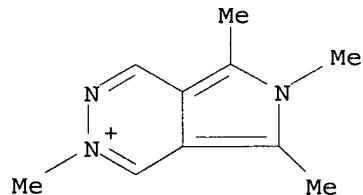
RN 30476-58-5 CAPLUS

CN 6H-Pyrrolo[3,4-d]pyridazine, 5,6,7-trimethyl- (8CI, 9CI) (CA INDEX NAME)



RN 79398-41-7 CAPLUS

CN 6H-Pyrrolo[3,4-d]pyridazinium, 2,5,6,7-tetramethyl-, iodide (9CI) (CA INDEX NAME)



● I<sup>-</sup>

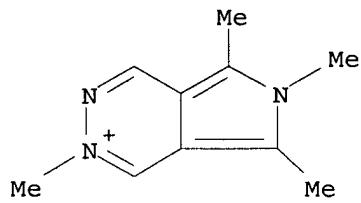
RN 79398-43-9 CAPLUS

CN 6H-Pyrrolo[3,4-d]pyridazinium, 2,5,6,7-tetramethyl-, sulfate (1:1) (CA INDEX NAME)

CM 1

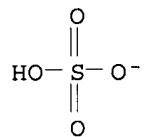
CRN 79398-42-8

CMF C10 H14 N3

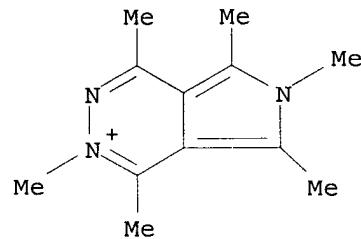


CM 2

CRN 14996-02-2  
CMF H O4 S

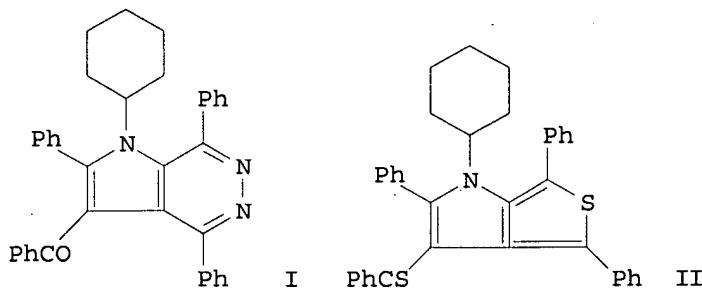


RN 79398-49-5 CAPLUS  
CN 6H-Pyrrolo[3,4-d]pyridazinium, 1,2,4,5,6,7-hexamethyl-, iodide (9CI) (CA INDEX NAME)



● I<sup>-</sup>

L9 ANSWER 14 OF 18 CAPLUS COPYRIGHT 2007 ACS on STN  
TI Synthetic approaches to fused heteroaromatic compounds by the condensation reactions of functional pyrroles  
GI



AB Diacyl- and triacylpyrroles, obtained by one pot synthesis from aziridines and acetylenic dipolarophiles, underwent condensation reactions. On treatment of 3,4-di- and 2,3,4-tribenzylopyrroles with hydrazine hydrate and phosphorus pentasulfide, pyrrolopyridazine derivs., e.g. I, and fused thiophenes, e.g. II, resp., were prepared. The structure proofs for I were based on the  $^{13}\text{C}$  FT-NMR spectrum of the corresponding  $^{13}\text{C}$ -enriched compds.

AN 1978:443293 CAPLUS <<LOGINID::20071212>>

DN 89:43293

OREF 89:6725a, 6728a

TI Synthetic approaches to fused heteroaromatic compounds by the condensation reactions of functional pyrroles

AU Uchida, Takane

CS Fac. Educ., Fukui Univ., Fukui, Japan

SO Journal of Heterocyclic Chemistry (1978), 15(2), 241-8

CODEN: JHTCAD; ISSN: 0022-152X

DT Journal

LA English

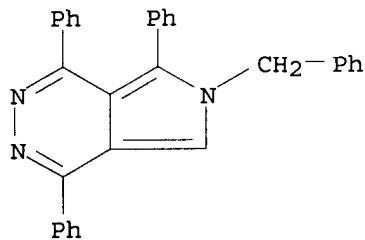
OS CASREACT 89:43293

IT 66864-43-5P 66864-44-6P 66939-89-7P

RL: SPN (Synthetic preparation); PREP (Preparation)  
(preparation of)

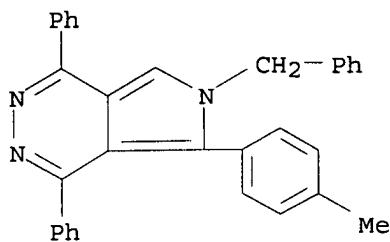
RN 66864-43-5 CAPLUS

CN 6H-Pyrrolo[3,4-d]pyridazine, 1,4,5-triphenyl-6-(phenylmethyl)- (CA INDEX NAME)



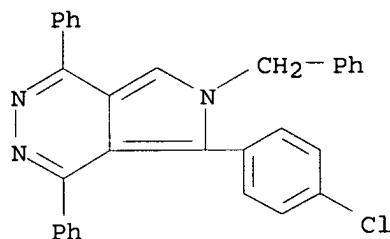
RN 66864-44-6 CAPLUS

CN 6H-Pyrrolo[3,4-d]pyridazine, 5-(4-methylphenyl)-1,4-diphenyl-6-(phenylmethyl)- (CA INDEX NAME)



RN 66939-89-7 CAPLUS

CN 6H-Pyrrolo[3,4-d]pyridazine, 5-(4-chlorophenyl)-1,4-dimethyl-6-(phenylmethyl)- (9CI) (CA INDEX NAME)



L9 ANSWER 15 OF 18 CAPLUS COPYRIGHT 2007 ACS on STN

TI Synthesis of new condensed pyrrolic heterocycles

GI For diagram(s), see printed CA Issue.

AB 1-Methyl-3,4-diformylpyrrole (I, R = CHO) (prepared by reduction of I (R = CO<sub>2</sub>Et) to give I (R = CH<sub>2</sub>OH) followed by oxidation with Ag<sub>2</sub>CO<sub>3</sub>) condensed with (MeO<sub>2</sub>CCH<sub>2</sub>)<sub>2</sub>CO, Et<sub>2</sub>CO, N<sub>2</sub>H<sub>4</sub>, and with H<sub>2</sub>NCH<sub>2</sub>CO<sub>2</sub>Et to give the condensed heterocycles II (R = CO<sub>2</sub>Me and Me) and III (X = N and CCO<sub>2</sub>Et), resp.

AN 1974:3411 CAPLUS <<LOGINID::20071212>>

DN 80:3411

OREF 80:595a, 598a

TI Synthesis of new condensed pyrrolic heterocycles

AU Duflos, J.; Letouze, D.; Queguiner, G.; Pastour, P.

CS Inst. Nat. Super. Chim. Ind., Rouen, Fr.

SO Tetrahedron Letters (1973), (36), 3453-4

CODEN: TELEAY; ISSN: 0040-4039

DT Journal

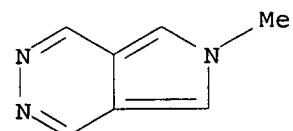
LA French

IT 51110-68-0P

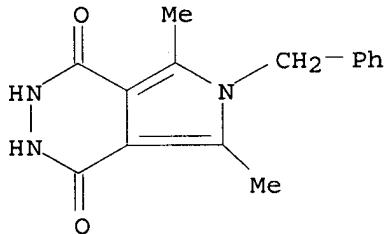
RL: SPN (Synthetic preparation); PREP (Preparation)  
(preparation of)

RN 51110-68-0 CAPLUS

CN 2H-Pyrrolo[3,4-d]pyridazine, 2-methyl- (9CI) (CA INDEX NAME)

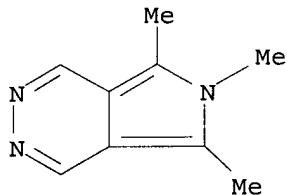


L9 ANSWER 16 OF 18 CAPLUS COPYRIGHT 2007 ACS on STN  
 TI Syntheses of pyridazino[1,2-a]pyridazine derivatives of furan, pyridazine, and pyrrole by Diels-Alder reactions  
 GI For diagram(s), see printed CA Issue.  
 AB Diels-Alder adducts were formed in the  $\text{Pb}(\text{OAc})_4$  oxidations of substituted cyclic hydrazides of furan, pyridazine, and pyrrole dicarboxylic acids in the presence of 1,3-cyclohexadiene or 1,3-cyclopentadiene. The products resulting were furo[3,4-g]pyridazino[1,2-a]pyridazine-6,10-diones (I), pyridazino[4,5-g]pyridazino[1,2-a]pyridazine-6,11-diones (II), and pyrrolo[3,4-g]pyridazino[1,2-a]pyridazine-6,10-diones (III), resp. Some hydrogenations and ring opening reactions were studied.  
 AN 1971:99966 CAPLUS <<LOGINID::20071212>>  
 DN 74:99966  
 OREF 74:16277a,16280a  
 TI Syntheses of pyridazino[1,2-a]pyridazine derivatives of furan, pyridazine, and pyrrole by Diels-Alder reactions  
 AU Gillis, Bernard T.; Valentour, James C.  
 CS Dep. Chem., Duquesne Univ., Pittsburgh, PA, USA  
 SO Journal of Heterocyclic Chemistry (1971), 8(1), 13-17  
 CODEN: JHTCAD; ISSN: 0022-152X  
 DT Journal  
 LA English  
 IT 31379-83-6P  
 RL: SPN (Synthetic preparation); PREP (Preparation)  
 (preparation of)  
 RN 31379-83-6 CAPLUS  
 CN 1H-Pyrrolo[3,4-d]pyridazine-1,4(6H)-dione, 6-benzyl-2,3-dihydro-5,7-dimethyl- (8CI) (CA INDEX NAME)



L9 ANSWER 17 OF 18 CAPLUS COPYRIGHT 2007 ACS on STN  
 TI Structure and reactivity of isocondensed heterocyclic systems with  $4n$  and  $(4m+2)$   $\pi$ -electrons. 2. Cyclizing condensation of 3,4-pyrroledicarboxaldehydes with compounds containing acidic CH and NH groups  
 GI For diagram(s), see printed CA Issue.  
 AB 6-Carbethoxy-1,2,3-trimethyl-2H-pyrrolo[3,4-c]-pyridine (I) is prepared by the reaction of 1,2,5-trimethyl-3,4-pyrroledicarboxaldehyde (II) with  $\text{H}_2\text{NCH}_2\text{CO}_2\text{Et}$ ; 1,2,3-trimethyl-2H-pyrrolo[3,4-d]pyridazine (III) is prepared from  $\text{N}_2\text{H}_4$ . II is treated with  $\text{RCH}_2\text{CH}_2\text{R}$  ( $\text{R} = \text{Bz, CN}$ ) to give the corresponding 2H-isoindoles (IV).  
 AN 1971:53695 CAPLUS <<LOGINID::20071212>>  
 DN 74:53695  
 OREF 74:8657a  
 TI Structure and reactivity of isocondensed heterocyclic systems with  $4n$  and  $(4m+2)$   $\pi$ -electrons. 2. Cyclizing condensation of 3,4-pyrroledicarboxaldehydes with compounds containing acidic CH and NH groups  
 AU Kreher, Richard; Vogt, Guenther  
 CS Inst. Org. Chem., Tech. Hochsch. Darmstadt, Darmstadt, Fed. Rep. Ger.  
 SO Angewandte Chemie, International Edition in English (1970), 9(12), 955-6  
 CODEN: ACIEAY; ISSN: 0570-0833  
 DT Journal

LA English  
 IT 30476-58-5P  
 RL: SPN (Synthetic preparation); PREP (Preparation)  
 (preparation of)  
 RN 30476-58-5 CAPLUS  
 CN 6H-Pyrrolo[3,4-d]pyridazine, 5,6,7-trimethyl- (8CI, 9CI) (CA INDEX NAME)



L9 ANSWER 18 OF 18 CAPLUS COPYRIGHT 2007 ACS on STN  
 TI Reactions of hydrazine with heterocyclic 1,2-dicarboxylic acid esters  
 AB The appropriate dicarboxylic acid ester (0.1 mol) in 25-50 cc. MeOH  
 treated with 15 g. N2H4.H2O, kept several hrs. at room temperature, heated 0.5  
 h. on the steam bath, and evaporated, the residue dissolved in 50-500 cc. H2O  
 containing 5 cc. concentrated NH4OH, the solution filtered and acidified with  
 excess  
 AcOH or HCl, and the crystalline precipitate washed and dried gave the  
 following  
 condensation products (m.p. and % yield given): 5,8-dihydroxy-1,4,6,7-  
 tetraazanaphthalene (I), 280° (decomposition), 95; 1,3-dimethyl-5,8-  
 dihydroxy-2,6,7-triazaanaphthalene, 302° (decomposition), 97; 2-NH2  
 derivative of I, above 400°, 93; 2-cyano-3-methyl-5,8-dihydroxy-4,6,7-  
 triazanaphthalene, 320° (decomposition), 85; 2-cyano-3,8-dimethyl-5-  
 hydroxy-4,6,7-triazaanaphthalene, 338-40°, 89; 1,4-dimethyl-5,8-  
 dihydroxy-2,3,6,7-tetraazanaphthalene, 320° (decomposition), 73;  
 4,7-dihydroxy-2-thia-5,6-diazaindene, 328-30°, 92;  
 2-methyl-4,7-dihydroxy-1-thia-5,6-diazaindene, 294-5°, 90;  
 1-methyl-4,7-dihydroxy-2-oxa-5,6-diazaindene (II), 282-3°, 77; 3-Me  
 derivative of II, 345° (decomposition), 83; 1-phenyl-2-methyl-4,7-dihydroxy-  
 1,5,6-triazaindene, 335-7°, 89; 1-phenyl-4,7-dihydroxy-1,2,5,6-  
 tetraazaindene, 315-16°, 61; 2-mercaptop-4,7-dihydroxy-1,3,5,6-  
 tetraazaindene (III), above 400°, 67; 1-methyl-4,7-dihydroxy-1,3,5,6-  
 tetraazaindene, 354-6°, 78°; 1-Me derivative of III, above  
 330°, 93; 1-phenyl-4,7-dihydroxy-1,3,5,6-tetraazaindene (IV),  
 315-16°, 89°; 2-SH derivative of IV, 367° (decomposition), 97.  
 The appropriate dicarboxylic dihydrazide (0.05 mol) refluxed 2-8 h. with  
 50 cc. N2H4.H2O or heated 9-72 h. on the steam bath, the solution evaporated in  
 vacuo on the steam bath, the solid residue dissolved in about 50-200 cc.  
 hot H2O, and the solution acidified with AcOH or HCl and cooled gave the  
 following condensation products (m.p. and % yield given):  
 2-methyl-4,7-dihydroxy-1-oxa-5,6-diazaindene (V), 290-2°, 96;  
 4,7-dihydroxy-2,5,6-triazaindene (VI), above 310°, 90; 2-Me derivative  
 (VII) of VI, 339-40°, 89; 1,5,6-isomer of V, 355°  
 (decomposition), -; 4,7-dihydroxy-1,3,5,6-tetraazaindene (VIII), above  
 400°, 92. The appropriate dihydrazide (0.05 mol) in 100 cc. 2N HCl  
 heated 6 h. on the steam bath, cooled, and filtered gave the following  
 condensation products: 4,7-dihydroxy-2-oxa-5,6-diazaindene, above  
 300°, 70; V; VI; VII; VIII. The appropriate diester (0.1 mol) in  
 about 50 cc. MeOH allowed to stand several hrs. with 15 g. N2H4.H2O or  
 heated 0.5 h. on the steam bath, and cooled, and the product recrystd.  
 from H2O or EtOH or dissolved in dilute acid and repptd. with NH4OH gave the  
 corresponding dicarboxylic acid dihydrazides (IX) of the following acids  
 (m.p. and % yield of the IX given): 4,5-imidazoledicarboxylic acid, above  
 375°, 99; 3,4-pyrazoledicarboxylic acid, above 300°, 98;

3,4-furandicarboxylic acid (X), 270° (decomposition), 88;  
 5-methyl-2,3-furandicarboxylic acid, m. 190°, 94;  
 3,4-pyrroledicarboxylic acid (XI), above 300°, 95; 1-Me derivative of XI, 330° (decomposition), 90. Dihydrazide of X (16 g.) and 25 cc. N2H4.H2O heated 6 h. on the steam bath, the brown solution evaporated in vacuo, the residue dissolved in 100 cc. dilute aqueous NaOH, and the solution treated

with

C and acidified with AcOH gave 13 g. 3,3'-dihydroxy-4,4'-bipyrazole (XII), darkened at 360° but did not melt (from H2O); XII was also obtained in 50% yield from di-Et 1-formyl-2-diethoxymethylsuccinate in EtOH with excess N2H4. 1-Methyl-4,7-dihydroxy-2-oxa-5,6-diazaindene (XIII) (10 g.) heated 8 h. on the steam bath with 20 cc. N2H4.H2O gave 90% 5-Me derivative of XII, m. above 360° (sublimed at 275° and 0.1 mm.). The 3-Me derivative of XIII gave similarly the 5,5'-di-Me derivative of XII, m. above 375°, in 52% yield when refluxed 15 h. with N2H4.

AN 1956:69457 CAPLUS <<LOGINID::20071212>>

DN 50:69457

OREF 50:13041a-h

TI Reactions of hydrazine with heterocyclic 1,2-dicarboxylic acid esters

AU Jones, Reuben G.

CS Lilly Research Labs., Indianapolis, IN

SO Journal of the American Chemical Society (1956), 78, 159-63

CODEN: JACSAT; ISSN: 0002-7863

DT Journal

LA Unavailable

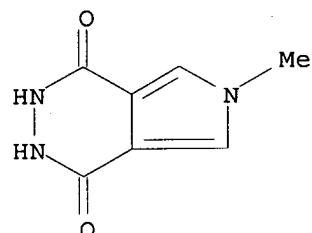
OS CASREACT 50:69457

IT 860362-71-6P, 6H-Pyrrolo[3,4-d]pyridazine-1,4-diol, 6-methyl-  
 RL: PREP (Preparation)

(preparation of)

RN 860362-71-6 CAPLUS

CN 6H-Pyrrolo[3,4-d]pyridazine-1,4-diol, 6-methyl- (5CI) (CA INDEX NAME)



=> d his

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FILE 'REGISTRY' ENTERED AT 10:19:12 ON 12 DEC 2007

L1 STRUCTURE UPLOADED

L2 0 S L1

L3 237 S L1 SSS FULL

FILE 'CAPLUS' ENTERED AT 10:21:22 ON 12 DEC 2007

L4 7 S L3

FILE 'REGISTRY' ENTERED AT 10:28:45 ON 12 DEC 2007

L5 STRUCTURE UPLOADED

L6 1 S L5

L7 86 S L5 SSS FULL

FILE 'CAPLUS' ENTERED AT 10:29:37 ON 12 DEC 2007

L8 19 S L7  
L9 18 S L8 NOT L4

=> log hold

COST IN U.S. DOLLARS	SINCE FILE ENTRY	TOTAL SESSION
FULL ESTIMATED COST	112.21	478.25
DISCOUNT AMOUNTS (FOR QUALIFYING ACCOUNTS)	SINCE FILE ENTRY	TOTAL SESSION
CA SUBSCRIBER PRICE	-16.38	-21.84

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LOGINID:SSPTAEX01623

PASSWORD:

\* \* \* \* \* RECONNECTED TO STN INTERNATIONAL \* \* \* \* \*  
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FULL ESTIMATED COST	112.21	478.25
DISCOUNT AMOUNTS (FOR QUALIFYING ACCOUNTS)	SINCE FILE ENTRY	TOTAL SESSION
CA SUBSCRIBER PRICE	-16.38	-21.84

=> file registry

COST IN U.S. DOLLARS	SINCE FILE ENTRY	TOTAL SESSION
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CA SUBSCRIBER PRICE	-16.38	-21.84

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DICTIONARY FILE UPDATES: 11 DEC 2007 HIGHEST RN 957570-32-0

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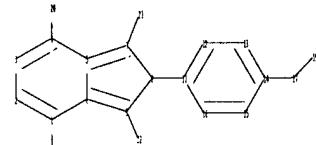
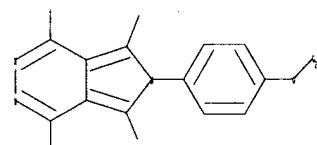
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<http://www.cas.org/support/stngen/stndoc/properties.html>

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ring nodes :  
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15-16  
exact/norm bonds :  
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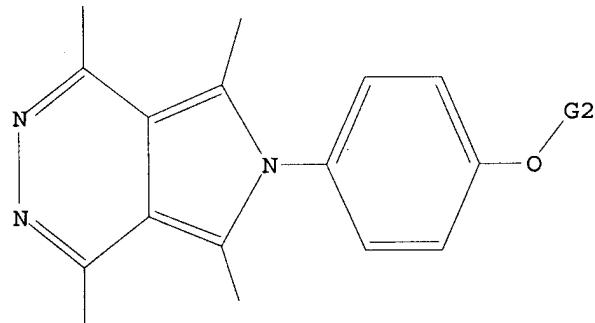
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G2:H,CH3,Et,n-Pr,i-Pr,CF3

Match level :  
1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 6:Atom 7:Atom 8:Atom 9:Atom 11:Atom  
12:Atom 13:Atom 14:Atom 15:Atom 16:Atom 17:CLASS 19:CLASS 20:CLASS 21:CLASS  
22:CLASS 23:CLASS

L10 STRUCTURE UPLOADED

=> d l10  
L10 HAS NO ANSWERS  
L10 STR



G1 H,Cy

G2 H,Me,Et,n-Pr,i-Pr,CF3

Structure attributes must be viewed using STN Express query preparation.

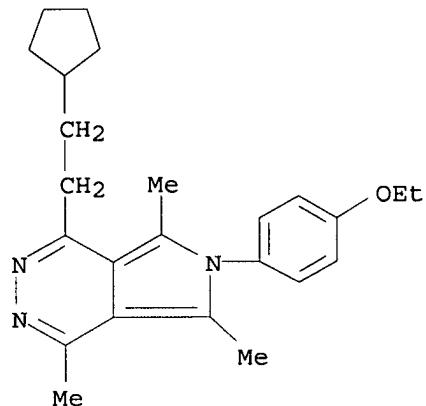
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SEARCH TIME: 00.00.01  
  
FULL FILE PROJECTIONS: ONLINE \*\*COMPLETE\*\*  
BATCH \*\*COMPLETE\*\*  
PROJECTED ITERATIONS: 2056 TO 3464  
PROJECTED ANSWERS: 3 TO 163

L11 3 SEA SSS SAM L10

=> d l11 scan

L11 3 ANSWERS REGISTRY COPYRIGHT 2007 ACS on STN  
IN 6H-Pyrrolo[3,4-d]pyridazine, 1-(2-cyclopentylethyl)-6-(4-ethoxyphenyl)-  
4,5,7-trimethyl-

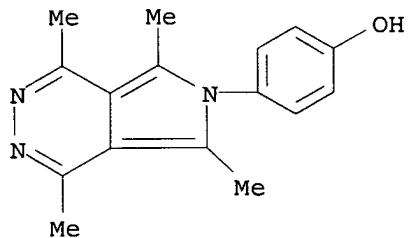
MF C24 H31 N3 O



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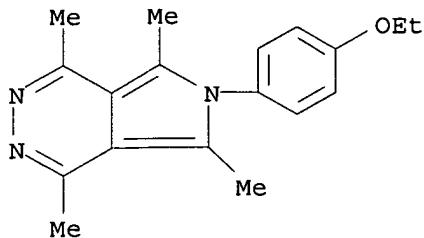
HOW MANY MORE ANSWERS DO YOU WISH TO SCAN? (1):2

L11 3 ANSWERS REGISTRY COPYRIGHT 2007 ACS on STN  
IN Phenol, 4-(1,4,5,7-tetramethyl-6H-pyrrolo[3,4-d]pyridazin-6-yl)-  
MF C16 H17 N3 O



\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

L11 3 ANSWERS REGISTRY COPYRIGHT 2007 ACS on STN  
IN 6H-Pyrrolo[3,4-d]pyridazine, 6-(4-ethoxyphenyl)-1,4,5,7-tetramethyl-  
MF C18 H21 N3 O



\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

ALL ANSWERS HAVE BEEN SCANNED

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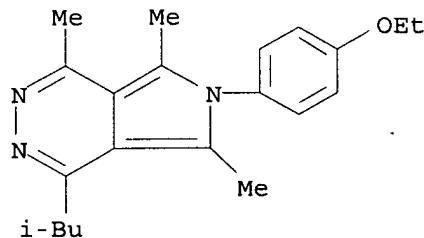
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54 ANSWERS

L12 54 SEA SSS FUL L10

=> d l12 scan

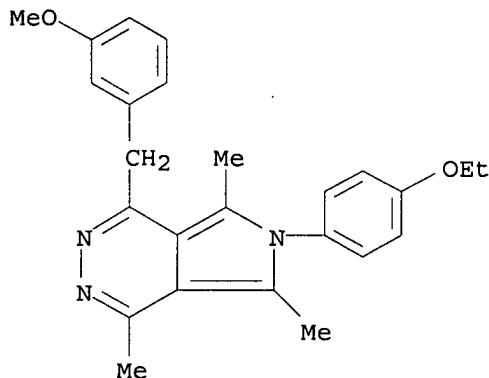
L12 54 ANSWERS REGISTRY COPYRIGHT 2007 ACS on STN  
 IN 6H-Pyrrolo[3,4-d]pyridazine, 6-(4-ethoxyphenyl)-1,5,7-trimethyl-4-(2-methylpropyl)-  
 MF C21 H27 N3 O



\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

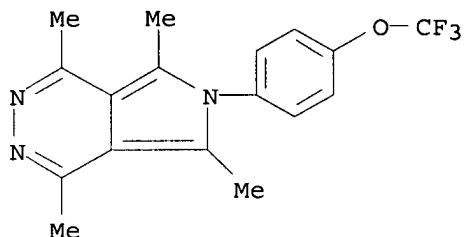
HOW MANY MORE ANSWERS DO YOU WISH TO SCAN? (1):2

L12 54 ANSWERS REGISTRY COPYRIGHT 2007 ACS on STN  
 IN 6H-Pyrrolo[3,4-d]pyridazine, 6-(4-ethoxyphenyl)-1-[(3-methoxyphenyl)methyl]-4,5,7-trimethyl-  
 MF C25 H27 N3 O2



\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

L12 54 ANSWERS REGISTRY COPYRIGHT 2007 ACS on STN  
 IN 6H-Pyrrolo[3,4-d]pyridazine, 1,4,5,7-tetramethyl-6-[4-(trifluoromethoxy)phenyl]-  
 MF C17 H16 F3 N3 O



\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

HOW MANY MORE ANSWERS DO YOU WISH TO SCAN? (1):0

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 'CPALUS' IS NOT A VALID FILE NAME  
 SESSION CONTINUES IN FILE 'REGISTRY'  
 Enter "HELP FILE NAMES" at an arrow prompt (=>) for a list of files  
 that are available. If you have requested multiple files, you can  
 specify a corrected file name or you can enter "IGNORE" to continue  
 accessing the remaining file names entered.

=> file caplus	SINCE FILE	TOTAL
COST IN U.S. DOLLARS	ENTRY	SESSION
FULL ESTIMATED COST	173.90	653.09
DISCOUNT AMOUNTS (FOR QUALIFYING ACCOUNTS)	SINCE FILE	TOTAL
CA SUBSCRIBER PRICE	ENTRY	SESSION
	0.00	-21.84

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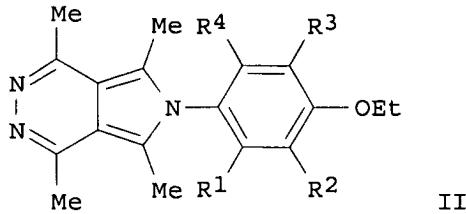
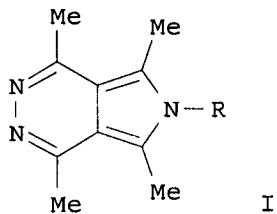
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L13 4 L12  
  
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L13 ANSWER 1 OF 4 CAPLUS COPYRIGHT 2007 ACS on STN  
TI Expedited SAR study of high-affinity ligands to the  $\alpha 2\delta$  subunit of voltage-gated calcium channels: Generation of a focused library using a solution-phase Sn2Ar coupling methodology  
AB The SAR of the lead compound 3, a novel ligand for the  $\alpha 2\delta$  subunit of voltage-gated calcium channels, was rapidly explored. Utilizing a parallel solution-phase Sn2Ar coupling approach, a focused library was obtained. The library was evaluated in vitro and afforded a series of analogs with improved potencies. The SAR trends of the library are also described.  
AN 2005:1342000 CAPLUS <<LOGINID::20071212>>  
DN 144:100381  
TI Expedited SAR study of high-affinity ligands to the  $\alpha 2\delta$  subunit of voltage-gated calcium channels: Generation of a focused library using a solution-phase Sn2Ar coupling methodology  
AU Chen, Chixu; Stearns, Brian; Hu, Tao; Anker, Naomi; Santini, Angelina; Arruda, Jeannie M.; Campbell, Brian T.; Datta, Purabi; Aiyar, Jayashree; Munoz, Benito  
CS Department of Chemistry, Merck Research Laboratories, San Diego, CA, 92121, USA  
SO Bioorganic & Medicinal Chemistry Letters (2006), 16(3), 746-749  
CODEN: BMCL8; ISSN: 0960-894X  
PB Elsevier B.V.  
DT Journal  
LA English  
OS CASREACT 144:100381  
RE.CNT 24 THERE ARE 24 CITED REFERENCES AVAILABLE FOR THIS RECORD  
ALL CITATIONS AVAILABLE IN THE RE FORMAT  
  
L13 ANSWER 2 OF 4 CAPLUS COPYRIGHT 2007 ACS on STN  
TI Synthesis and biological evaluation of 6-aryl-6H-pyrrolo[3,4-d]pyridazine derivatives as high-affinity ligands of the  $\alpha 2\delta$  subunit of voltage-gated calcium channels  
GI



AB 2H-pyrrolo[3,4-c]pyridazines I (R = 4-EtOC<sub>6</sub>H<sub>4</sub>, 2-EtO-5-pyridinyl, 5-EtO-2-pyridinyl, 5-EtO-2-pyrazinyl, 4-EtO-1-pyridazinyl, 2-EtO-5-pyrimidinyl, etc.) such as II (R<sub>1</sub> = H, MeO, Et, H<sub>2</sub>C:CH, Me, MeS, EtO, F; R<sub>2</sub> = H, Me; R<sub>3</sub> = H, Me, Cl, HOCH<sub>2</sub>; R<sub>4</sub> = H, Me) are prepared as ligands for the  $\alpha$ 2 $\delta$  subunit of voltage-gated calcium channels. Ortho-substituents capable of electron-donation increase the binding of II to the  $\alpha$ 2 $\delta$  subunit of voltage-gated calcium channels; electron-withdrawing substituents in the ortho-position of II decrease binding significantly. II (R<sub>1</sub> = MeO; R<sub>2</sub> = R<sub>3</sub> = R<sub>4</sub> = H) binds to the  $\alpha$ 2 $\delta$  subunit of voltage-gated calcium channels from A710 cells with an IC<sub>50</sub> value of 4 nM. Testing of tritiated ligand II (R<sub>1</sub> = TCH<sub>2</sub>TCH; R<sub>2</sub> = R<sub>3</sub> = R<sub>4</sub> = H) in purified human  $\alpha$ 2 $\delta$  voltage-gated calcium channel subunits indicates that II displace Gabapentin from the  $\alpha$ 2 $\delta$  subunit of voltage-gated calcium channels, and thus act as Gabapentin mimics in vitro. In the preparation of II (R<sub>1</sub> = Et; R<sub>2</sub> = R<sub>3</sub> = R<sub>4</sub> = H), a novel metal-free hydrogenation is used using hydrazine as the reductant; the reduction is effective in other systems (no data).

AN 2004:303255 CAPLUS <>LOGINID::20071212>>

DN 141:54277

TI Synthesis and biological evaluation of 6-aryl-6H-pyrrolo[3,4-d]pyridazine derivatives as high-affinity ligands of the  $\alpha$ 2 $\delta$  subunit of voltage-gated calcium channels

AU Hu, Tao; Stearns, Brian A.; Campbell, Brian T.; Arruda, Jeannie M.; Chen, Chixu; Aiyar, Jayashree; Bezverkov, Robert E.; Santini, Angelina; Schaffhauser, Herve; Liu, Wensheng; Venkatraman, Shankar; Munoz, Benito

CS MRLSDB2, Department of Medicinal Chemistry, Merck Research Laboratories, San Diego, CA, 92121, USA

SO Bioorganic & Medicinal Chemistry Letters (2004), 14(9), 2031-2034  
CODEN: BMCLE8; ISSN: 0960-894X

PB Elsevier Science B.V.

DT Journal

LA English

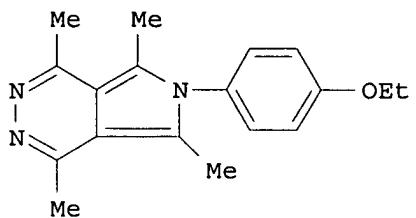
OS CASREACT 141:54277

RE.CNT 9 THERE ARE 9 CITED REFERENCES AVAILABLE FOR THIS RECORD  
ALL CITATIONS AVAILABLE IN THE RE FORMAT

L13 ANSWER 3 OF 4 CAPLUS COPYRIGHT 2007 ACS on STN

TI Synthesis and biological evaluation of 6-aryl-6H-pyrrolo[3,4-d]pyridazine derivatives: high-affinity ligands to the  $\alpha$ 2 $\delta$  subunit of voltage gated calcium channels

GI



I

AB A novel class of 6-aryl-6H-pyrrolo[3,4-d]pyridazine ligands for the  $\alpha 2\delta$  subunit of voltage-gated calcium channels has been described. Substitutions in the aryl ring of the mol. were generally not tolerated, and resulted in diminished binding to the  $\alpha 2\delta$  subunit. Modifications to the pyridazine ring revealed numerous permissive substitutions, and detailed SAR studies were carried out in this portion of the mol. Replacement of the pyridazine ring Me group with an aminomethyl functionality provided greatly improved potency over the initial lead. The initial lead compound (I) displayed good rat pharmacokinetic properties, and was shown to be efficacious in the Chung model for neuropathic pain in rats.

AN 2004:153601 CAPLUS <<LOGINID::20071212>>

DN 140:357282

TI Synthesis and biological evaluation of 6-aryl-6H-pyrrolo[3,4-d]pyridazine derivatives: high-affinity ligands to the  $\alpha 2\delta$  subunit of voltage gated calcium channels

AU Stearns, Brian A.; Anker, Naomi; Arruda, Jeannie M.; Campbell, Brian T.; Chen, Chixu; Cramer, Merryl; Hu, Tao; Jiang, Xiaohui; Park, Kenneth; Ren, Kun Kun; Sablad, Marciano; Santini, Angelina; Schaffhauser, Herve; Urban, Mark O.; Munoz, Benito

CS Department of Medicinal Chemistry, Merck Research Laboratories, San Diego, CA, 92121, USA

SO Bioorganic & Medicinal Chemistry Letters (2004), 14(5), 1295-1298  
CODEN: BMCL8; ISSN: 0960-894X

PB Elsevier Science B.V.

DT Journal

LA English

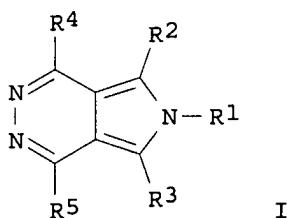
OS CASREACT 140:357282

RE.CNT 16 THERE ARE 16 CITED REFERENCES AVAILABLE FOR THIS RECORD  
ALL CITATIONS AVAILABLE IN THE RE FORMAT

L13 ANSWER 4 OF 4 CAPLUS COPYRIGHT 2007 ACS on STN

TI Treatment of neuropathic pain with 6H-pyrrolo[3,4-d]pyridazine compounds

GI



AB The title compds. [I; R1 = (un)substituted alkyl(hetero)aryl, alkyl(hetero)cycloalkyl, (hetero)aryl, (hetero)cycloalkyl; R2-R5 = a bond, (un)substituted alkyl, alkyl(hetero)aryl, alkyl(hetero)cycloalkyl, (hetero)aryl, (hetero)cycloalkyl] were prepared as ligands of voltage

gated calcium channels (VGCC), useful in the treatment of neuropathic pain, and psychiatric and mood disorders such as, for example, schizophrenia, anxiety, depression, panic, and bipolar disorder, as well as in the treatment of pain, Parkinson's disease, cognitive dysfunction, epilepsy, circadian rhythm disorders, drug addiction, drug abuse, drug withdrawal and other. E.g., a multi-step synthesis of I [R1 = 4-EtOC6H4; R2-R4 = Me; R5 = 4-MeOC6H4] which produced a 65% effect after i.p. dosing at 30 mg/kg in spinal nerve ligation model of neuropathic pain in rats, was given. The pharmaceutical composition comprising the compound I is claimed.

AN 2004:60243 CAPLUS <<LOGINID::20071212>>

DN 140:111422

TI Treatment of neuropathic pain with 6H-pyrrolo[3,4-d]pyridazine compounds  
IN Anker, Naomi Burke; Arruda, Jeannie M.; Campbell, Brian Thomas; Munoz, Benito; Prasit, Petpiboon; Stearns, Brian A.

PA Merck & Co., Inc., USA

SO PCT Int. Appl., 203 pp.

CODEN: PIXXD2

DT Patent

LA English

FAN.CNT 1

	PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI	WO 2004006836	A2	20040122	WO 2003-US21493	20030708
	WO 2004006836	A3	20040415		
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	EP 1539168	A2	20050615	EP 2003-764414	20030708
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PRAI	US 2002-394734P	P	20020711		
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OS	MARPAT 140:111422				